Minimising the Expected Posterior Entropy Yields Optimal Summary Statistics

Till Hoffmann and Jukka-Pekka Onnela
{thoffmann, onnela}@hsph.harvard.edu
Harvard T. H. Chan School of Public Health, Boston, MA

Extracting low-dimensional summary statistics from large datasets is essential for efficient (likelihood-free) inference. We characterise different classes of summaries and demonstrate their importance for correctly analysing dimensionality reduction algorithms. We propose obtaining summaries by minimising the expected posterior entropy (EPE) under the prior predictive distribution of the model. Many existing methods are equivalent to or are special or limiting cases of minimising the EPE. We develop a method to obtain high-fidelity summaries that minimise the EPE; we apply it to benchmark and real-world examples. We both offer a unifying perspective for obtaining informative summaries and provide concrete recommendations for practitioners.

1 Introduction

Empowered by advances in both scientific understanding and computing, researchers are developing ever more sophisticated simulators. For example, simulated weak lensing maps capture how dark matter affects light propagating through the universe [1, 2], coalescent simulators predict the evolution of genetic material [3], and synthetic networks shed light on political opinion formation [4], effective vaccination strategies [5], as well as interactions between proteins [6].

While simulators can quickly generate data y given parameters θ, we are often interested in the inverse problem: Constraining parameters θ in light of a dataset y. If the likelihood g(y | θ) is available, we can use Markov chain Monte Carlo samplers [7] or variational inference [8, Ch. 10] to investigate the posterior distribution f(θ | y). But inference is more challenging if the likelihood is not tractable or is too costly to evaluate.

Approximate Bayesian computation (ABC) overcomes this challenge in three steps by comparing the observed data with synthetic data [9]: First, we draw a large number of
samples (θ, z_i) from the prior predictive distribution which form the so-called reference table. Second, we evaluate the distance d_i = d(y, z_i) between the observed data y and the ith synthetic dataset z_i. Finally, we accept θ_i as a sample from the approximate posterior f(θ | y) if the distance d_i to the observed data is smaller than some threshold ϵ. The smaller ϵ, the better the posterior approximation. Intuitively, ABC draws parameter samples θ_i that generate synthetic data z_i which “look like” the observed data y. For the remainder of the manuscript, we will use z to denote simulated data and reserve y for observed data.

Unfortunately, ABC and more recent likelihood estimation networks [10] suffer from the curse of dimensionality: The larger the dataset, the larger the number of simulations required to obtain a sample that satisfies d_i < ϵ. Compressing the data to lower-dimensional summary statistics t = t(y) (or summaries in short) can overcome the curse of dimensionality but leaves us with the question: How do we choose the compression function t(y)?

A plethora of methods has been developed to address this question, some of which are summarised in panel (a) of Fig. 1. They include subset selection methods which select informative summaries from a pool of candidates [11, 12, 13, 14, 15] as well as parameterised transformations that can be optimised to learn summaries [16, 17, 18, 19, 20, 21, 22]. Loss functionals that quantify how well the compressor preserves information have been motivated by minimising the Bayes risk [17, 19], model selection [1, 18, 23], and information theoretic arguments [13, 14, 21, 22]. These methods all seek to address the same challenge. How might they be related?

After formalising the notion of different summaries in Section 2, we argue that all information-theoretic approaches are equivalent in Section 3: They implicitly minimise the same loss functional between the posterior f(θ | t) given only summaries t and the full posterior f(θ | y) given the entire dataset y. While these results are well established in information theory, they provide a unifying perspective of different summary extraction approaches. Minimising the expected posterior entropy (EPE) should be the practitioner’s choice because it is straightforward to evaluate compared with the Kullback-Leibler divergence or mutual information, especially in high dimensions. It also has strong connections with recent advances in conditional posterior density estimation [24, 25]. But even methods developed to address different problems (such as parameter inference or model selection) in diverse fields (such as cosmology or population genetics), have strong ties to information-theoretic approaches. For example, in Section 4 we show that maximising the determinant of the Fisher information [21, 26] and minimising the L^2 Bayes risk [17, 19] are both equivalent to minimising the EPE in the large-sample limit. Similarly, learning a probabilistic classifier for model selection [18] minimises the EPE. In Section 5, we discuss concrete steps for learning informative summaries by fitting flexible conditional posterior density estimators to simulated data. To compare different methods, we devise a benchmark problem with simple likelihood but data that prove challenging for summary selection in Section 5.1. We also compare different summary selection approaches on two applied examples: Inferring the mutation and recombination rates of a population genetics model (Section 5.2) and inferring the attachment kernel for a model of growing trees (Section 5.3).
Figure 1: Different methods for compressing data to informative summaries are intimately related; distinguishing between classes of summaries is essential. Panel (a) illustrates that five information-theoretic approaches (ITAs) are equivalent: They implicitly minimise the same loss functional (Sections 2 and 3). Approximate sufficiency (Section 4.1) seeks to achieve lossless compression, and minimising the posterior entropy (Section 4.2) is a special case of ITAs focused on only the observed data. Maximising the Fisher information (Section 4.3) and minimising the $L^2$ Bayes risk (Section 4.4) are equivalent to one another as well ITAs in the large-sample limit. Probabilistic model selection (Section 4.6) maps onto ITAs if we treat model labels as parameters to be inferred. A dashed arrow from one method to another indicates that the latter is a specialisation of the former, and solid arrows indicate correspondence in the large-sample limit. Panel (b) illustrates relationships between classes of summaries. Sufficient statistics $S$ are a subset of lossless statistics $L$ although the former only exist if the likelihood belongs to the exponential family. The intersection of $L$ and the space of summaries $T$ considered by the practitioner are optimal summaries $O$. In general, optimal summaries need not be lossless such that $O \cap L = \emptyset$, e.g. if $T$ is restricted to a certain parametric transformation.
2 Background

Given data \( y \) we would like to infer parameters \( \theta \) of a model using summaries \( t = t(y) \) that retain as much information about the posterior distribution as possible. Summaries \( t_{\text{suff}} \) with fixed and finite dimensions are Bayes sufficient if \( f(\theta \mid t_{\text{suff}}) = f(\theta \mid y) \) for all \( y \) and any prior \( \pi(\theta) \) [27]. But they only exist for exponential-family likelihoods [28].

We thus have to relax the concept of sufficiency, and we say that the statistics \( t_{\text{lossless}} \) are lossless if
\[
f(\theta \mid t_{\text{lossless}}(y)) = f(\theta \mid y)
\]
for all parameter values \( \theta \), all data \( y \) of the same sample size, and a given prior \( \pi(\theta) \).

While lossless statistics always exist (e.g. the identity map) they may not be useful in practice, and we say that the statistics \( t_{\text{opt}} \) are optimal if they minimise a non-negative loss functional \( \ell \) which measures the discrepancy between the posterior given the entire dataset and the posterior given only the summaries. Loss functionals include, for example, the Kullback-Leibler divergence, Wasserstein distance, and total variation distance [29]. In particular,
\[
t_{\text{opt}} = \arg\min_{t \in \mathcal{T}} \ell \{ f(\theta \mid y), f(\theta \mid t(y)) \},
\]
where \( \mathcal{T} \) is the space of summaries under consideration, and the loss functional \( \ell \) is zero if and only if the statistics are lossless. Consequently, sufficient statistics are lossless, and lossless statistics are optimal, but the converse is not necessarily true. For example, \( \mathcal{T} \) may be restricted to a certain parametric transformation [17] or selecting at most \( k \) summaries from a set of candidate statistics [23], possibly leading to information loss.

The relationship between different classes of summaries is illustrated in panel (b) of Fig. 1.

Despite the pursuit of the holy grail of sufficient statistics, most applications will have to settle for the weakest concept of optimal statistics. Even the most sophisticated method cannot extract sufficient statistics if the likelihood does not belong to the exponential family [28]. Similarly, unless the family of summaries \( \mathcal{T} \) is rich enough, lossless compression is not achievable. Furthermore, even if \( \mathcal{T} \) is rich enough, one cannot in general verify that Eq. (1) holds for all \( \theta \) and \( y \) given a finite computational budget.

While models with exponential-family (conditional) likelihoods are theoretically appealing, they may not be sufficiently expressive or intuitive to address real-world problems. Domain knowledge can aid in the development of powerful models that capture salient features of the data, including protein interaction networks [6], cosmology [21], and population-genetics [3]. But these models often do not have sufficient statistics or even tractable likelihoods, and we need to resort to possibly lossy compression and likelihood-free inference.

3 Minimising the expected posterior entropy

We propose choosing the summaries such that the expected posterior entropy (EPE) is minimised, where the expectation is taken with respect to the prior predictive dis-
tribution of the generative model, similar to the evaluation of the Fisher information [8, Ch. 6]. This approach is conceptually simple and computationally tractable, has a strong connection with recent inference techniques based on conditional density estimation [24, 25], and is equivalent to other information-theoretic approaches, as illustrated in panel (a) of Fig. 1.

Recall that the posterior entropy given summaries \( t(z) \) for a fiducial dataset \( z \) is

\[
H \{ f(\theta \mid t(z)) \} = -\int d\theta f(\theta \mid t(z)) \log f(\theta \mid t(z)).
\]

Taking the expectation with respect to the data under the generative model yields the EPE

\[
\mathcal{H} \equiv \mathbb{E}_{z \sim p(z)} [H \{ f(\theta \mid t(z)) \}] = -\int dt \int d\theta p(t, \theta) \log f(\theta \mid t(z)),
\]

where \( p(z) = \int d\theta g(z \mid \theta) \pi(\theta) \) is the marginal likelihood, and \( \mathbb{E}_{z \sim p(z)} [\cdot] \) denotes the expectation with respect to \( z \) under the distribution \( p(z) \). Changing variables of integration from data \( z \) to summaries \( t \) leaves us with the simple expression

\[
\mathcal{H} = -\int dt \int d\theta p(t, \theta) \log f(\theta \mid t),
\]

where the Jacobian has been absorbed by the joint density \( p(t, \theta) \). With a slight abuse of notation, we use \( p(\cdot) \) for both the marginal likelihood and joint distribution where the distinction is unambiguous. Given a conditional density estimator \( \hat{f}(\theta \mid t) \) that seeks to approximate the posterior, we can construct a Monte Carlo estimate of the EPE

\[
\hat{\mathcal{H}} = -m^{-1} \sum_{i=1}^{m} \log \hat{f}(\theta_i, t(z_i)),
\]

where \( \theta_i \) and \( z_i \) are joint samples from \( p(\theta, z) \), and \( m \) is the number of samples. This Monte Carlo estimate is in fact the widely employed loss function for learning the posterior from simulated data [24, 25], where \( m \) is the size of the mini-batch, i.e. a subset of the data used to evaluate gradients for training the model.

We consider three well-established connections to other information-theoretic approaches although with a specific focus on the selection of summaries for ABC [8, Ch. 1]. First, we evaluate the difference between the prior entropy and EPE

\[
H \{ \pi(\theta) \} - \mathcal{H} = \int dt \int d\theta f(\theta \mid t) \log \left( \frac{f(\theta \mid t)}{\pi(\theta)} \right),
\]

where we have been able to combine the two integrals because

\[
\int d\theta \pi(\theta) \log \pi(\theta) = \int dt \int d\theta p(t, \theta) \log \pi(\theta)
\]

by the law of total probability. The inner integral of Eq. (5) is the Kullback-Leibler divergence from the prior to the posterior \( D_{KL}(f(\theta \mid t) \parallel \pi(\theta)) \), sometimes called surprise.
because it measures the degree to which an observer updates their belief in light of new data [30]. Minimising the EPE thus maximises our expected surprise from observing the summaries because the prior entropy does not depend on the choice of summaries.

Second, we note that \( f(\theta | t) = p(t, \theta) / \pi(t) \) and Eq. (5) simplifies to the mutual information between the summaries \( t \) and parameters \( \theta \)

\[
I(\theta, t) = \int dt d\theta p(t, \theta) \log \left( \frac{p(\theta, t)}{\pi(\theta) p(t)} \right).
\]

As the mutual information is non-negative, the EPE is not larger than the prior entropy, i.e. we reduce uncertainty on average. Minimising the EPE is equivalent to maximising the mutual information which has been proposed in the context of subset selection [14] and, more recently, neural summaries [22]. However, estimating mutual information is a difficult task in high dimensions [31], making the approach computationally challenging.

Third, we consider the difference between the EPE given only summaries \( t \) and the EPE given a full fiducial dataset \( z \)

\[
\mathcal{H} - \mathbb{E}_{z \sim p(z)} [H \{ f(\theta | z) \}] = \int dz p(z) \int d\theta f(\theta | z) \log \left( \frac{f(\theta | z)}{f(\theta | t)} \right),
\]

and we can identify the inner integral as the Kullback-Leibler divergence from \( f(\theta | t) \) to \( f(\theta | z) \) (see App. 8 for details). The difference of expected entropies is thus equal to the expected Kullback-Leibler divergence between the posteriors

\[
\mathcal{H} - \mathbb{E}_{z \sim p(z)} [H \{ f(\theta | z) \}] = \mathbb{E}_{z \sim p(z)} [D_{KL}(f(\theta | z) \parallel f(\theta | t))],
\]

which Chan et al. [20] considered in the context of inferring recombination hotspots in population genetics. Minimising the EPE is equivalent to minimising the expected Kullback-Leibler divergence because the posterior entropy given the complete dataset does not depend on the choice of summaries. The Kullback-Leibler divergence is non-negative which allows us to draw two conclusions. First, the posterior entropy given only summaries \( t(z) \) is greater than or equal to the posterior entropy given the full dataset \( z \), i.e. we lose information in expectation by conditioning on the summaries instead of the complete dataset unless the summaries are lossless. Second, minimising the EPE implies that the loss functional in Eq. (2) is the expected Kullback-Leibler divergence. Similar to the mutual information, evaluating the expected Kullback-Leibler divergence is computationally challenging and neither \( f(\theta | z) \) nor \( f(\theta | t) \) are known in practice.

To summarise, minimising the EPE, maximising the mutual information between parameters \( \theta \) and summaries \( t \), maximising the expected surprise, and minimising the expected Kullback-Leibler divergence between \( f(\theta | z) \) and \( f(\theta | t) \) are all equivalent. But minimising the EPE should be the practitioner’s choice because it can be estimated easily using Eq. (4) for functional approximations of the posterior and nearest-neighbour entropy estimators for posterior samples [32].
4 Related work and connections with expected posterior entropy

4.1 Approximate sufficiency

Joyce and Marjoram [12] cast the task of selecting summaries as a sequence of hypothesis tests to select a subset of candidate summaries. Specifically, they consider the log ratio

$$\log R_k(\theta) = \log f(\theta | t_k, \ldots, t_1) - \log f(\theta | t_{k-1}, \ldots, t_1),$$

where $f(\theta | t_{k-1}, \ldots, t_1)$ is the approximate posterior distribution given $k-1$ summaries currently included in the subset of “interesting” statistics, and $f(\theta | t_k, \ldots, t_1)$ is the posterior resulting from including an additional candidate statistic $t_k$. Intuitively, if the error score $\delta_k = \max_\theta |\log R_k(\theta)|$ is zero, i.e. the two posteriors are identical, the $k^{th}$ statistic does not provide any additional information and can be ignored. If $\delta_k$ differs significantly from zero, we reject the null hypothesis that $f(\theta | t_k, \ldots, t_1)$ and $\log f(\theta | t_{k-1}, \ldots, t_1)$ are the same distribution and add $t_k$ to the selected summaries.

However, the error score $\delta_k = \max_\theta |\log R_k|$ can have surprising properties because considering the maximum assigns equal importance to all subsets of the parameter space—even regions that we know to be irrelevant. For example, suppose that the posterior given the currently selected $k-1$ summaries is normal with variance $\sigma^2_{k-1}$, and the posterior after adding the $k^{th}$ summary is identical except for a different variance $\sigma^2_k$. Even if $\sigma_k$ and $\sigma_{k-1}$ differ by an infinitesimal amount, $\delta_k$ is unbounded because

$$\delta_k = \frac{1}{2} \max_\theta \left| \log \left( \frac{\sigma^2_k}{\sigma^2_{k-1}} \right) + \left( \frac{\sigma^2_{k-1} - \sigma^2_k}{\sigma^2_k \sigma^2_{k-1}} \right) \sigma^2 \right| = \infty.$$

The error score is dominated by regions of the parameter space that have virtually no posterior mass. The expected value $\mathbb{E}_{\theta \sim f(\theta | t_k, \ldots, t_1)} [\log R_k(\theta)]$ instead weights discrepancies between the two distributions by the posterior mass. This quantity is in fact the Kullback-Leibler divergence considered by Barnes et al. [14] (see Section 4.5 for details).

Joyce and Marjoram [12] employed a histogram density estimator to compare the two approximate posteriors $f(\theta | t_k, \ldots, t_1)$ and $f(\theta | t_{k-1}, \ldots, t_1)$. They consider a candidate statistic $t_k$ informative if the number of samples in any histogram bin differs significantly between the two posteriors according to a $z$-test.

The notion of “approximate” sufficiency is necessarily a statement about limited computational resources: If we had unlimited computational resources, only candidate statistics that are uninformative or redundant would be excluded. This observation applies more generally to any subset selection algorithm, such as minimising posterior entropy [13] in Section 4.2, regression-based subset selection methods [11, 15] in Section 4.4, or maximising mutual information [14] in Section 4.5.

4.2 Minimising the conditional posterior entropy

Nunes and Balding [13] proposed choosing a subset of summaries $t$ by minimising the conditional posterior entropy (CPE) $H \{ f(\theta | t(y)) \}$ given a particular observed dataset.
They ran rejection ABC for different subsets of summaries and evaluated the CPE using a nearest-neighbour estimator [32]. The proposal is appealing because low-entropy posteriors give precise parameter estimates.

However, it implicitly assumes that the data we have observed are the only data that could ever be observed—similar to the non-parametric bootstrap. When the maximum likelihood estimate of the parameters lies in the tail of the prior distribution, the CPE $H \{ f (\theta | y) \}$ can be larger than the prior entropy $H \{ \pi (\theta) \}$ because the posterior is a “compromise” between prior and likelihood [15].

We consider a simple example with closed form posterior because it highlights important concepts and intuitively illustrates challenges associated with learning informative summaries. Suppose we draw $n = 4$ samples $y$ from a zero-mean normal distribution with precision (inverse variance) $\theta$ which we would like to infer. We use a gamma distribution prior for $\theta$ because it is the conjugate prior for a normal likelihood with known mean. The distribution is parameterised by a shape or concentration parameter $a$ and inverse scale or rate parameter $b$. We use $b = 1$ throughout such that the prior mean is $a$. More formally,

$$
\theta \mid a, b \sim \text{Gamma} (a, b) \tag{7}
$$

$$
y_i \mid \theta \sim \text{Normal} (0, \theta^{-1}) ,
$$

where $i \in \{1, \ldots, n\}$. The closed-form posterior is

$$
\theta \mid y, a, b \sim \text{Gamma} \left( a + \frac{n}{2}, b + \frac{nt}{2} \right) ,
$$

where $t = n^{-1} \sum_{i=1}^{n} y_i^2$ is the second moment of the data and a sufficient statistic for a normal likelihood with known mean. For example, if $a = 1.5$ and $t = 0.3$, the prior entropy is 1.36 and the CPE is 1.47. Minimising the CPE would discard the sufficient statistic $t$ such that the posterior is equal to the prior—we have not learned anything from the data. Panel (a) of Fig. 2 shows the entropy gain $\Delta = H \{ f (\theta | y) \} - H \{ \pi (\theta) \}$ in light of the data for different priors and sample variances. Indeed, generating data from the prior predictive distribution with $a = 1.5$, we find that 30% of samples lead to a CPE increase. Interestingly, this situation is more likely to arise when the “surprise” [30] is large, and we should substantially update our beliefs in light of the data. In contrast, the EPE $H = 0.87$ given $t$ is smaller than the prior entropy, and minimising it would select $t$ as a useful summary. We estimated the EPE and proportion of entropy increases by drawing $10^5$ samples from the generative model. Monte Carlo standard errors are smaller than the reported significant digits.

Nunes and Balding [13] also considered a two-stage method: First they employed the minimum CPE approach to select candidate summaries and identify simulated datasets close to the observed data. Second, they drew posterior samples for each identified dataset and evaluated the root mean integrated squared error (RMISE) of posterior
Figure 2: Selecting or learning summaries can be non-trivial even for toy models. Panel (a) shows the difference between posterior and prior entropy for a model with zero-mean normal likelihood and conjugate gamma prior for the precision $\theta$ (inverse variance). For a subset of the parameter and data space, minimising the posterior entropy would discard the second moment $t$, which is a sufficient statistic. Panel (b) shows the bimodal posterior distribution for the example point in (a) that arises when the precision of the likelihood is $|\theta|$, as discussed in Section 4.4. The posterior mean is zero and not informative of the parameter. The vertical dashed line represents the maximum likelihood estimate $|\theta|$ of the precision $|\theta|$.
samples for each subset of summaries. This is possible because the parameters of simulated datasets are known. The summaries with the lowest RMISE were then selected. We do not consider this two-stage approach further here because of its computational burden and because posterior mean estimation methods optimise a similar objective, as discussed in Section 4.4.

4.3 Maximising the Fisher information

Even when the likelihood is tractable, compressing the data $y$ to summaries $t$ can have computational benefits. Heavens, Jimenez, and Lahav [26] developed an optimal linear compression scheme for Gaussian likelihoods in the sense that the Fisher information is preserved. Information-maximising neural networks [21] seek to maximise the Fisher information when linear compression is not sufficient, and methods to maximise the Fisher information for non-Gaussian likelihoods have recently been developed [2, 33].

We consider the large-sample limit $n \to \infty$ such that, according to the Bernstein–von Mises theorem, the posterior approaches a multivariate normal distribution under certain regularity conditions which we will consider in more depth [34]. Specifically,

$$
\theta \mid t \sim \text{Normal} \left( \theta_0, F^{-1}(\theta_0) \right),
$$

where $\theta_0$ is the true parameter that generated the summaries $t$, and

$$
F_{ij}(\theta_0) = \mathbb{E}_{z \sim p(z)} \left[ \left( \frac{\partial}{\partial \theta_i} \log g(t(z) \mid \theta) \right) \left( \frac{\partial}{\partial \theta_j} \log g(t(z) \mid \theta) \right) \right]_{\theta=\theta_0}
$$

is the Fisher information of the summaries evaluated at $\theta_0$ [8, Ch. 6]. The limiting entropy of the posterior can thus be readily evaluated and is

$$
\lim_{n \to \infty} H \{ f(\theta \mid t) \} = -\frac{1}{2} \log \det F(\theta_0) + \text{constant},
$$

where $\det F$ denotes the determinant of $F$. We take the expectation with respect to the prior $\pi$ to obtain the EPE

$$
\lim_{n \to \infty} \mathcal{H} = -\frac{1}{2} \int d\theta_0 \, \pi(\theta_0) \log \det F(\theta_0) + \text{constant}.
$$

We do not need to take an expectation with respect to the summaries $t \mid \theta_0$ because the Fisher information defined in Eq. (8) is itself an expectation and does not depend on the realisation $t$. Maximising the expected log determinant of the Fisher information matrix is thus equivalent to minimising the EPE in the large-sample limit. This observation agrees with our intuition that the effect of the prior on the posterior decreases as the sample size increases—at least for simple models.

We argue that minimising the EPE is more appealing than maximising the Fisher information for three reasons. First, it can incorporate prior information in the small-$n$ regime to yield the most faithful posterior approximation. Second, it does not require the choice of a fiducial value of $\theta$ at which to evaluate the Fisher information. Finally,
when the likelihood is not available, we need to approximate it to evaluate the Fisher information. For example, Charnock, Lavaux, and Wandelt [21] assume that the likelihood of the learned summaries can be approximated by a Gaussian, and Alsing and Wandelt [33] argue that candidate summaries often have a Gaussian likelihood if they are the mean of i.i.d. data.

4.4 Minimising the Bayes risk

Fearnhead and Prangle [17] proposed the posterior mean of the parameters as a summary. Of course, the posterior mean is not known, but we can estimate it by minimising the quadratic loss

\[ \ell = E_{z, \theta \sim p(z, \theta)} \left[ (\theta - t_\beta(z))^T A (\theta - t_\beta(z)) \right] \] (9)

where \( t_\beta(z) \) is a predictor of \( \theta \) parameterised by \( \beta \), \( A \) is a positive-definite matrix, \( A \) denotes the transpose, and the expectation is taken with respect to the joint distribution \( p(z, \theta) \). Fearnhead and Prangle [17] considered linear predictors, but neural networks [19] and boosted regression [16] have also been employed to estimate the posterior mean. In practice, the parameters \( \beta \) are learned by minimising a Monte Carlo estimate of Eq. (9) akin to Eq. (4). Using the estimated posterior mean \( t_\beta(\cdot) \) as summaries implicitly chooses as many summaries as there are parameters.

Considering again the large-sample limit, the quadratic loss becomes (adapted from Theorem 3 of Fearnhead and Prangle [17])

\[ \ell = \text{tr} \left[ A \int d\theta \pi(\theta) F^{-1}(\theta) \right] , \]

where \( \text{tr} \) denotes the matrix trace. Consequently, minimising the quadratic loss in Eq. (9) is intimately related to maximising the determinant of the Fisher information because both \( A \) and \( F \) are positive-definite. However, the details depend on the form of \( A \).

The above argument crucially depends on the assumptions of the Berstein–von Mises theorem holding. In particular, the model needs to be identifiable such that different values of the parameters \( \theta \) are distinguishable in the \( n \to \infty \) limit [34]. We consider a simple variant of the toy model presented in Section 4.2 that is not identifiable and discuss the impact on learning summaries. In particular, we use the absolute value \( |\theta| \) of a parameter \( \theta \) as the precision such that the conditional distributions are

\[ \theta \mid a, b \sim u \times \text{Gamma} (a, b) \]

\[ y_i \sim \text{Normal} \left( 0, |\theta|^{-1} \right) , \]

where \( u \) is \( \pm 1 \) with equal probability. The posterior is

\[ \theta \mid y, a, b \sim u \times \text{Gamma} \left( a + \frac{n}{2}, b + \frac{nt}{2} \right) , \]

where \( t \) is the second moment of the data as in Eq. (7) and a sufficient statistic. The posterior distribution is bimodal and symmetric under reflection, as shown in panel (b) of
Fig. 2. Importantly, the posterior mean is zero, and any attempt to extract information by minimising Eq. (9) will fail.

This example may seem contrived, and, in this case, the problem can be resolved by switching back to the original parameterisation. But multimodal posteriors that render the posterior mean uninformative are not uncommon. For example, mixture models are invariant under label permutation [35], and latent-space models of networks [36] as well as latent factor models for Bayesian PCA [37] are invariant under rotations. More generally, point estimates are problematic if the likelihood is invariant under a transformation but the estimate is not. Using information theoretic approaches ensures we stay focused on the task at hand: Approximating the posterior.

The relationship between parameters and data can be complex, and regression approaches, especially linear regression, may not be able to capture the relationship globally. Local relationships in regions of high posterior mass can be learned using pilot runs [17] or weighting samples [11]. Local regression methods have also been adapted for subset selection: A model is fit to predict parameters from candidate summaries, and a candidate is selected if it increases a metric such as the Bayesian evidence [11], Akaike information criterion, or Bayesian information criterion [15].

4.5 Maximising the mutual information

Barnes et al. [14] proposed choosing summaries from a pool of candidates that maximise the mutual information $I\{\theta, t\}$ between parameters $\theta$ and the statistics $t$. Assuming that the candidate set includes sufficient statistics $t_{\text{suff}}$ such that

$$f(\theta \mid t_{\text{suff}}) = f(\theta \mid y) \quad (10)$$

for all possible $y$, they constructed a set of summaries sequentially. At the $k^{\text{th}}$ step, they included the summary that maximises the surprise given the $k - 1$ statistics that have already been selected. The approach is similar to the approximate sufficiency method reviewed in Section 4.1, but candidates are prioritised by their surprise at each stage. Together, the steps select the summaries that maximise the surprise $D_{\text{KL}}(f(\theta \mid t) \parallel \pi(\theta))$.

However, recall from Eqs. (5) and (6) that the mutual information is equal to the expected surprise under the generative model. In general, maximising the surprise for a particular observed dataset is thus not equivalent to maximising the mutual information. The approach may select different summaries if the candidate set does not include sufficient statistics.

Similarly, Chen et al. [22] sought to maximise the mutual information using a neural network. They suggested that “$t(z)$ is a sufficient statistic for $g(z \mid \theta)$ if and only if” (p. 2) it maximises the mutual information and “that the sufficiency of the learned statistics is insensitive to the choice of $\pi(\theta)$” (p. 4) such that “[their approach] is globally sufficient for all $\theta$” (p. 6). As we shall illustrate with a toy model, these propositions do not hold in general because of the difference between sufficient and optimal statistics discussed in Section 2 (see App. 9 for details).

\[1\]We have adapted notation in quotations for consistency with this manuscript.
Figure 3: Optimal summaries depend on the prior. Panel (a) shows the parameters of a piecewise likelihood with qualitatively different behaviour on either side of the transition at $\theta = 0$. Panel (c) shows two priors with the bulk of their mass on either side of the transition. Panels (b) and (d) show the relationship between the parameter and the sample mean $\bar{y}$ and log variance $\log \text{var} y$, respectively, as a scatter plot. Mutual information estimates highlight that the optimal choice of summary depends on the prior: The $\bar{y}$ and $\log \text{var} y$ summaries are informative for the priors centred at +1 and −1, respectively.
Consider the piecewise likelihood
\[
y_i \mid \theta = \begin{cases} 
\text{Normal}(0, \exp \theta) & \text{if } \theta < 0 \\
\text{Normal}(\theta, 1) & \text{if } \theta \geq 0
\end{cases}
\] (11)
which is continuous at the transition, as illustrated in panel (a) of Fig. 3. We consider two different normal priors with common standard deviation of 0.25 centred at ±1, as shown in panel (c). For the purpose of this example, we may choose one summary from the candidate set comprising the sample mean \(\bar{y}\) and the natural logarithm of the sample variance \(\log \text{var } y\), i.e. we restrict the space of compression functions \(T^2\). Intuitively, the latter is informative for the “left” region of the parameter space and the former for the “right”. This intuition is confirmed by simulation: We consider \(m = 10^5\) independent samples from each prior and draw \(n = 100\) observations from the likelihood in Eq. (11). The relationship between the parameter \(\theta\) and sample mean as well as log sample variance are shown in panels (b) and (d), respectively. For quantitative comparison, we also estimate the mutual information for all pairs of priors and summaries using a nearest-neighbour entropy estimator [32] by noting that
\[
I\left\{t, \theta\right\} = H\{\pi(\theta)\} + H\{p(t)\} - H\{p(t, \theta)\}.
\]
On the one hand, the log sample variance (\(I = 0.70\)) is the optimal summary for the left prior because the sample mean provides little information (\(I = 0.02\)). On the other hand, the sample mean is highly informative for the right prior (\(I = 0.98\)) whereas the log sample variance is not informative (\(I = 0.00\)). As Bayesians, we cannot escape the prior, and the optimal summaries depend on it.

4.6 Model selection
Prangle et al. [18] used logistic regression to learn summaries that can discriminate between different models: The predicted class probabilities. Similarly, Merten et al. [1] applied deep convolutional neural networks to weak lensing maps to learn features that can discriminate between nine different cosmological models—although not in the context of ABC. Such probabilistic approaches to model classification are equivalent to minimising the EPE: Consider a one-hot encoding of the model index such that \(\theta_j = 1\) if model \(j\) generated the data and \(\theta_j = 0\) otherwise. The log posterior is thus
\[
\log f(\theta \mid t) = \sum_{j=1}^{r} \theta_j \log f(\theta_j = 1 \mid t),
\] (12)
where \(r\) is the number of models under consideration, and \(f(\theta_j = 1 \mid t)\) is the posterior probability that the data were generated by model \(j\). Equation (12) is immediately familiar as the negative cross-entropy loss widely used for multiclass classification in machine learning [8, Ch. 4]. In other words, any machine learning classifier that minimises the cross-entropy loss for model selection minimises the EPE of the model labels.

\footnote{We restrict \(T\) to simplify the example. Together, the two summaries are sufficient. A continuous mixture of the “left” and “right” part of the likelihood with logistic mixture weight would yield similar results but does not have sufficient statistics.}
4.7 Conditional posterior density estimation

As briefly discussed in Section 3, recent approaches to likelihood-free inference based on conditional density estimation minimise the EPE using the mini-batch estimator in Eq. (4) as a loss function [24, 25]. These methods are appealing because they can automatically compress large datasets although at the cost of having to choose an architecture for the density estimator which is an active area of research [38]. Chan et al. [20] proposed exchangeable neural networks such that the output is invariant under permutations of i.i.d. data generated by the model. While neural density estimators can in principle learn such invariances, it is beneficial to encode symmetries in the architecture to improve efficiency and reduce the amount of training data required. In practice, conditional density estimators can have computational advantages over rejection ABC because they interpolate the posterior density in the parameter space, requiring fewer simulations [24]. However, they cannot offer the same asymptotic guarantees as ABC: As the tolerance parameter of the acceptance kernel is reduced, the sampling distribution converges to the true posterior [9].

4.8 Further methods

Burr and Skurikhin [39] sought to extract summaries ensuring that the approximate posterior is well calibrated, i.e. the true parameter used to generate synthetic data is contained within the \( \alpha \)-credible interval of the corresponding approximate posterior for a fraction \( \alpha \) of simulations. Calibration is a necessary condition for reliable inference [40], but it is not sufficient to choose summaries. For example, discarding all data yields perfect calibration because the posterior is equal to the prior. We do not consider the method further here.

Wegmann, Leuenberger, and Excoffier [41] obtained summaries using partial least squares regression (PLSR), a latent variable model for supervised dimensionality reduction. The method projects data \( z \) (or candidate summaries) to a latent space such that the embeddings are most predictive of the parameters \( \theta \) as measured by the \( L_2 \) norm. Instead of the predictions of the model as in Section 4.4, the latent variables are used as summaries. The number of latent components is chosen using leave-one-out cross-validation based on the ability of the model to predict parameters. Similar to the subset selection methods discussed in Sections 4.1 and 4.2, the number of components chosen by cross-validation is determined by computational constraints: For sufficiently large reference tables, the dimensionality of the candidate summaries is maintained provided each candidate summary encodes some information, however weak.

5 Experiments

We consider three experiments to compare different methods for extracting summaries from varied datasets: A benchmark model with i.i.d. observations and tractable likelihood in Section 5.1, a population genetics model with data comprising candidate summaries in Section 5.2, and a model of growing trees in Section 5.3. We first discuss
Figure 4: Mixture density networks with a bottleneck can learn informative summaries. The left section illustrates the training procedure: $p$-dimensional parameters $\theta$ and synthetic data $z$ are drawn from the prior $\pi$ and simulator $g$, respectively. Synthetic data are compressed to summaries using a neural compressor $t$, and a mixture density network (MDN) $h$ estimates a posterior approximation $\hat{f}(\theta \mid t(z))$, where $F$ are the supported posteriors, e.g. MDNs with certain component distributions. The density estimate is scored using the negative log probability (NLP) loss and the network is optimised by minimising it. The right section illustrates approximate Bayesian computation using learned summaries: The trained compressor evaluates summaries of observed data $y$, and parameter samples are accepted if the corresponding simulated summaries $t(z)$ are sufficiently close to the observed summaries $t(y)$. The table lists the type of data $D$ and compressor architecture for each experiment (see Sections 5.1 to 5.3 for details).
the overarching approach for consistently evaluating summary extraction methods on qualitatively different datasets and subsequently consider each experiment in depth.

For subset selection methods (such as minimising the CPE in Section 4.2) and simple projections (such as linear posterior mean estimation in Section 4.4 or PLS in Section 4.8), we evaluated candidate summaries that were supplied to each algorithm to extract the most informative summaries. For more flexible nonlinear posterior mean estimation, we developed experiment-specific neural compressors $t : \mathbb{D} \rightarrow \mathbb{R}^q$ to compress the raw data $z \in \mathbb{D}$ to $q$ low-dimensional summaries. The networks were trained by minimising the quadratic loss in Eq. (9).

Summaries minimising the EPE are appealing, but a concrete algorithm is required to make them useful in practice. We employed a conditional mixture density network (MDN) [24] with a bottleneck akin to an autoencoder [42]. A similar approach was used by Jeffrey, Alsing, and Lanusse [31] for summaries fed to a likelihood estimation network. The network comprises two parts: First, for fair comparison, we used the same neural compressor as for nonlinear posterior mean estimation. Consequently, the number of summaries $q$ is equal to the number of parameters $p$, although, in general, a different number of summaries $q > p$ could be chosen [22]. Second, we extended the network with a conditional MDN to estimate the posterior density given only the summaries. The composite network was trained by minimising the Monte Carlo estimate of the EPE defined in Eq. (4). After training, the bottleneck architecture ensures any information that may be useful for minimising the EPE is captured by the output of the compressor; we dub this approach MDN compression. The inference pipeline is illustrated in Fig. 4.

For each experiment, we generated a training, validation, and test set by sampling from the prior predictive distribution. Neural compressors were trained by mini-batch gradient descent using the Adam optimiser with default parameters and an initial learning rate of $10^{-2}$ [43]. The learning rate was decreased by an order of magnitude if the loss evaluated on the validation set did not decrease for ten consecutive epochs; training was stopped if it did not decrease for twenty consecutive epochs.

After extracting summaries for each example in the test set, we obtained samples from the approximate posterior distribution $f(\theta \mid t(y))$ in two steps: First, we standardised summaries to ensure a common scale and evaluated the Euclidean distance $d(t(y), t(z_i))$ between each example $y$ and the $i^{th}$ element of the training set $z_i$. Second, we accepted a small fraction of the reference table as posterior samples such that they had the smallest distance to each example [9], i.e. the training set served as the reference table. In addition to ABC, we drew samples from the prior as a baseline as well as directly from the MDNs trained to obtain EPE-minimising summaries.

We used two metrics to evaluate approximate posterior samples. First, the root mean integrated squared error (RMISE)

$$\text{RMISE} = \left[ \frac{1}{s} \sum_{i=1}^{s} \left\| \hat{\theta}_i - \theta \right\|^2 \right]^{1/2},$$

where $\hat{\theta}_i$ denotes the $i^{th}$ sample from the approximate posterior, and $s$ is the number of approximate posterior samples. This metric has been widely used in the ABC literature
to evaluate summary extraction methods [12, 13, 15, 17, 19, 39]. It measures how concentrated approximate posterior samples are around the true parameter value $\theta$ [8, Ch. 3]. While Eq. (13) is a biased estimate of the RMISE due to the nonlinear square root transform, we are only concerned with the relative performance of different approaches here such that the bias is immaterial. The RMISE is a suitable metric for unimodal but not multimodal posteriors, as illustrated in panel (b) of Fig. 2. Second, to address this shortcoming, we also evaluated the negative log probability (NLP) using Gaussian kernel density estimation. It is defined as

$$\text{NLP} = -\log \left[ \frac{1}{s} \sum_{i=1}^{s} K_\sigma \left( \tilde{\theta}_i - \theta \right) \right],$$

(14)

where $K_\sigma$ is a Gaussian kernel with bandwidth $\sigma$ chosen by Scott’s rule [44].

5.1 Benchmark model

We considered a benchmark model with multimodal posterior set up to be challenging for extracting summaries. The model has a tractable likelihood that allowed us to compare the approximate posterior given summaries with exact posterior samples. In particular, we sampled a univariate parameter $\theta$ from the standard normal distribution and drew $n = 10$ independent samples from the mixture distribution

$$y_i \mid \theta \sim \begin{cases} \frac{1}{2} \sum_{u \in \{-1,1\}} \text{Normal} \left( u \times \tanh \theta, 1 - \tanh^2 \theta \right), \\
\end{cases}$$

as illustrated in panel (a) of Fig. 5. We also sampled a standard normal distractor (uninformative noise) for each observation $i$ such that the full dataset $Y$ is a matrix with $n$ rows and 2 columns. Learning or selecting summaries is non-trivial because all elements of $Y$ have zero mean and unit variance under the generative model irrespective of the parameter $\theta$. The first moment is zero by symmetry; the second moment of each mixture component is

$$\mathbb{E} \left[ y^2 \right] = \mathbb{E} \left[ y^2 \right] + \text{var} \ y = \tanh^2 \theta + 1 - \tanh^2 \theta = 1$$

such that the mixture has unit variance. Sampling from the prior predictive distribution, we generated training, validation, and test sets of $10^6$, $10^4$, and $10^3$ independent realisations, respectively. The test set was used to evaluate and compare different methods. We employed the likelihood-based inference framework Stan [7] to draw $1,000$ posterior samples for each example in the test set (see App. 10 for details). These samples formed the “ground truth” which we compared other methods to.

For ABC using candidate summaries, the CPE minimisation method [13], PLS [41], and linear posterior mean estimation [17], we used the first three even moments of each column of $Y$ as initial or candidate summaries, giving rise to six statistics in total. Odd moments are not informative since the likelihood is symmetric, and we did not include them in our set of candidate summaries.

For the nonlinear posterior mean approximation [19], we used a simple multilayer perceptron (MLP) that acts on each row of $Y$ independently before compressing the dataset to a scalar summary. This architecture shares weights across all observations.
Figure 5: A conditional mixture density network (MDN) that minimises the expected posterior entropy learns highly informative summaries. Panel (a) shows the likelihood for a particular parameter value $\theta_0 \approx 1.6$ together with a rug plot for $n = 10$ samples $y_0$. Panel (b) shows the exact posterior $f(\theta | y)$ given the data in (a) together with the learned mixture density. While the two-component mixture is not flexible enough to approximate the posterior well, it learns highly informative summaries: MDN-compressed ABC samples using these summaries are shown as a histogram. Panel (c) shows the learned summary $t(\cdot)$; markers correspond to the data in (a). The dashed line is a fit to the learned summaries based on the first three even moments of $y$. Panel (d) illustrates the relationship between the mixture density approximation and the summary as a heat map; lighter colours indicated higher posterior density.
and is permutation invariant [20]. The MLP has three fully connected layers (16, 16, and 1 hidden units) followed by mean-pooling across the $n$ observations; we used tanh activation functions between layers throughout. The network was implemented in PyTorch [45] and trained as described in the preceding section with a mini-batch size of 512.

Finally, we employed a conditional MDN with $k = 2$ Gaussian components to estimate the posterior and learn MDN-compressed summaries [24, 46]. To evaluate the mixture logits $\eta(t)$, locations $\mu(t)$, and log-scales $\kappa(t)$ as a function of the summary $t$ we used independent two-layer MLPs (16 and $k$ hidden layers). The approximate posterior is thus

$$
\hat{f}(\theta \mid t) = \sum_{j=1}^{k} \text{softmax}_j(\eta(t)) \times \text{Normal}(\theta \mid \mu_j(t), \exp(\kappa_j(t)),$$

where $\text{softmax}_j(\eta) = \exp(\eta_j) / \sum_{i=1}^{k} \exp(\eta_i)$.

A comparison of the performance of different methods based on 1,000 approximate posterior samples (0.1% of the reference table) is shown in panel (a) of Fig. 6 (see Table 1 in the appendix for a table of results). We report the RMISE for completeness, but it is a poor metric for multimodal posteriors. For example, a point mass at $\theta = 0$ would have RMISE = 1—lower than any of the methods we considered. As expected, linear and nonlinear posterior mean estimators performed worst in terms of NLP because the posterior is bimodal. Because of its flexibility, the nonlinear estimator was able to accurately estimate the posterior mean $E_{\theta \sim f(\theta \mid z)}[\theta] = 0$ which, ironically, led to the worst performance: The NLP is equal to the prior entropy (1.42). The linear estimator performed better because the regression coefficients are entirely determined by noise in the training set, i.e. the scalar summary is a random projection of the candidate summaries. Similarly, extracting features using PLS regression is driven by noise: Here, three random orthogonal projections of candidate features were selected based on five-fold cross-validation, allowing PLS to outperform both linear and nonlinear regression. Minimising the conditional posterior entropy and using candidate summaries without selection performed similarly and better than regression-based approaches.

MDN-compressed ABC performed almost as well as the gold standard likelihood-based inference and better than samples drawn directly from the MDN, as illustrated in panel (b) of Fig. 5 for a particular example. The architecture of the MDN is too restrictive to provide a good posterior approximation. Increasing the number of components to $k = 10$ provides a better approximation (NLP = 1.05 ± 0.01) with the same performance as both the likelihood-based approach and MDN-compressed ABC. Here, we deliberately restricted the architecture to illustrate that ABC with good summaries can remain competitive because it does not rely on parametric assumptions about the density.

Due to the simplicity of the benchmark problem, we can inspect the properties of the MDN and the learned summary, as shown in panel (c). The appropriate summary is obvious in retrospect: It should discriminate between data $y$ clustered around ±1 (corresponding to large absolute values of $\theta$) and data near zero or large absolute value (corresponding to small absolute values of $\theta$). A linear fit based on the candidate
Figure 6: The quality of summaries has a significant impact on the fidelity of posteriors. Panels (a), (b), and (c) report the negative log probability loss (NLP) and root mean integrated squared error (RMISE) of different summary extraction methods for the benchmark, coalescent, and growing tree experiments, respectively. Error bars are standard errors based on a test set of 1,000 independent samples for each experiment. Expert summaries and PLS perform relatively poorly for the growing tree experiment and are indicated as off-the-chart by arrows.
summaries illustrates that they are rich enough to provide a high-quality summary in principle, but most methods struggled to extract the information. We obtained the fit by minimising squared residuals on the interval \((-3, 3)\) weighted by the prior density. Finally, the density of the MDN, shown in panel (d), exhibits the expected behaviour: Large summaries give rise to unimodal distributions centred at the origin, whereas small summaries yield bimodal posterior approximations.

The choice of compressor architecture is not unique. For example, we could have included further layers after the mean-pooling operation or used a fully-connected network throughout. However, using the mean-pooled latent features has a unique advantage: They are unbiased estimates of the population mean of the features independent of sample size. The architecture was motivated by the observation that the likelihood of exponential family distributions can be expressed in terms of sums (or means) of transformations of the data. We thus expect the learned summaries to remain informative for different sample sizes. To test this hypothesis, we repeated the analysis with \(n = 100\) instead of \(n = 10\) observations per example. The NLPs are smaller because we had access to more data: 0.68 ± 0.01 for likelihood-based inference and 0.70 ± 0.01 for MDN-compressed ABC, where the MDN was trained on the larger dataset using the same methodology as before. Running MDN-compressed ABC with the network trained on the smaller dataset yielded a NLP of 0.72 ± 0.01, i.e. the performance is almost indistinguishable from the network trained on the larger dataset despite being exposed to an order of magnitude fewer observations. Importantly, the MDN itself cannot achieve this generalisation because the model was trained on data with a fixed sample size.

5.2 Population genetics model

As a more applied example, we inferred the mutation and recombination rates of a population genetics model—a problem that has been extensively studied using ABC in general and in the context of identifying informative summaries in particular [12, 13, 15]. The data were generated using the coalescent approach which considers the history of a sample of haplotypes, a set of DNA variations that tend to be inherited together because they are close together on the DNA strand. This approach yields a powerful perspective for both analytical study of population genetics as well as simulation [3]. However, we present the process in terms of the equivalent forward model here because it is more accessible. Under the neutral Fisher-Wright model, a large population of diploid organisms (each having paired chromosomes) reproduces sexually in discrete generations without selection pressure. Haplotypes are subject to random mutations under an infinite-sites assumption, i.e. the DNA sequence is sufficiently long that the probability of multiple mutations occurring at the same site is negligible. The model also allows for recombination, i.e. the haplotype of a gamete can be a combination of parental haplotypes. We consider a finite-sites recombination model [47], i.e. the strands may only cross over at specific locations during meiosis. This may seem at odds with the infinite-sites mutation model, but we can think of the haplotype as a sequence of atomic segments, each comprising a very large number of bases. See Nordborg [3] for a more comprehensive discussion.
We used a dataset of $10^6$ simulations from the above model generously provided by Nunes and Balding [13]. The rate at which mutations and recombination occurs in the population were drawn independently from a uniform distribution on the interval $(0, 10)$ which also served as the prior for inference. For each simulation, 50 haplotypes with 5,001 base pairs were generated. Seven candidate summaries comprised a uniform distractor and six expert summaries (such as the number of unique haplotypes or “the frequency of the most common haplotype” (p. 8); see Nunes and Balding [13] for details). We split the dataset into training, validation, and test sets comprising $9.89 \times 10^5$, $10^4$, and $10^3$ samples, respectively.

For the non-linear regression model, we used a three-layer MLP with 16, 16, and 2 hidden units. Mean-pooling was not required because the input to the neural network was a set of candidate statistics. We employed the same architecture for the compressor of the mixture density network. Instead of two Gaussian components, we used ten beta distributions rescaled to the interval $(0, 10)$ as component distributions. We used the same architecture as in Section 5.1 to estimate the mixture logits and the logarithm of the beta shape parameters. Both networks were trained as previously described with mini-batch size of 256.

We drew 1,000 posterior samples for each example in the test set (comprising $\approx 0.1\%$ of the reference table as for the benchmark dataset). Kernel density estimates of the NLP are biased for bounded parameters because probability mass can “leak” out of the support [44]. We used a reflection-based bias correction technique to estimate the NLP [48], i.e. each approximate posterior sample $\tilde{\theta}$ in Eq. (14) is reflected at the boundaries such that both tails of the kernel contribute to the density estimate. The results are shown in panel (b) of Fig. 6 and Table 1 in the appendix. Nonlinear regression and MDN-compressed ABC not only performed comparably, but the two methods also learned very similar summaries: After standardising and aligning the summaries using a Procrustes transformation [49], they had a pointwise MSE of $M^2 = 0.20$ ($p$-value $< 10^{-3}$ under a permutation test). MDN samples performed slightly, but not statistically significantly, better in terms of EPE and RMISE. The minimum CPE method performed worst in terms of NLP because it targets highly concentrated posteriors, but they may not be concentrated near the true parameter value. We did not implement the two-stage method of [13] due to its computational cost and similarity with posterior mean estimation approaches [17, 19]. Similarly, we omitted approximate sufficiency [12] because it is sensitive to the number of histogram bins chosen for density estimation and is not suitable for multidimensional parameter spaces due to the curse of dimensionality.

### 5.3 Growing tree model

Inferring the parameters of dynamic network models is challenging, especially when only cross-sectional data are available. Cantwell, St-Onge, and Young [50] developed a pseudo-marginal Markov chain Monte Carlo (PM-MCMC) algorithm to infer the parameters of a growing tree model, e.g. to study phylogenetic trees or infection traces. Under the model [51], a tree is grown starting with a single isolated node. At each step, a new node $j$ is added to the tree, and it connects to an existing node $i$ with probability $\propto k_i^j$, 

where $k_i$ is the degree of node $i$, i.e. the number of connections it has. The parameter $\theta$ controls the strength of preferential attachment: The larger $\theta$ the more likely nodes are to connect to nodes that already have many connections. The likelihood is intractable because the history, i.e. the order of addition of nodes, is unknown. There are combinatorially many possible histories to consider such that evaluating the likelihood exactly is prohibitively expensive save for very small trees. The PM-MCMC algorithm estimates the marginal likelihood by sampling a set of histories consistent with the observed graph and averaging the conditional likelihood given each history [50].

Here, we employed ABC to infer the preferential attachment parameter $\theta$ and compared different methods to extract informative summaries from graph data. Synthetic data were generated by sampling the kernel parameter $\theta$ from a uniform distribution $\text{Uniform}(0, 2)$ and simulating trees with $n = 100$ nodes for each kernel parameter. Unlike the two previous experiments with $10^6$ records in the reference table, we generated a training set of $10^5$ samples for performance reasons. The validation and test sets both comprised $10^3$ samples.

For subset selection methods, we used one uniform distractor and four candidate summaries we expected to be informative of $\theta$: The standard deviation and Gini coefficient of the degree distribution because heavy-tailed degree distributions are indicative of large $\theta$; the diameter of the network and the maximum betweenness centrality because the existence of a central hub connecting disparate parts of the tree is indicative of large $\theta$ [52]. For nonlinear posterior mean estimation and MDN compression, we used a two-layer graph isomorphism network (GIN) where each layer comprised a two-layer MLP with eight hidden units per layer [53]. We used the constant vector of ones as input features for the GIN because nodes are indistinguishable. Features were mean-pooled across the graph after applying the GIN, and the networks were trained with 32 trees per mini-batch.

All methods, including using candidate summaries directly, were able to significantly reduce uncertainty about the attachment parameter compared with the prior. As shown in panel (c) of Fig. 6 and Table 1 in the appendix, the PM-MCMC algorithm had the lowest RMISE, but MDN-compressed ABC and direct sampling from the MDN performed best as measured by NLP. Similar to the benchmark experiment in Section 5.1, we repeated the experiment for larger trees with $n = 748$ nodes. MDN compression trained on large trees performed best (NLP = $-1.67 \pm 0.02$), but the summaries learned on trees with $n = 100$ nodes generalised to the larger dataset with NLP = $-1.65 \pm 0.02$. The relative NLP performance of other methods remained unchanged, but PM-MCMC performance was sensitive to the size of the grown tree and degraded severely with NLP = 1.7$\pm$0.2 much larger than the prior entropy $H \{ \pi(\theta) \} = 0.69$. For superlinear preferential attachment, i.e. $\theta > 1$, almost every newly added node connects to a central hub [51]. This phenomenon is particularly pronounced for larger graphs, and it is challenging to infer histories accurately which leads to poor posterior inference. In this experiment, ABC with MDN-compressed summaries outperformed the dedicated (pseudo-marginal) likelihood-based approach.
6 Discussion

We have shown that five information-theoretic approaches to devising summaries are equivalent in Section 3. Furthermore, as shown in Section 4, other methods can be understood as special or limiting cases of minimising the expected posterior entropy (EPE) which should be the practitioner’s choice because it is straightforward to evaluate compared with mutual information or Kullback-Leibler divergence, can incorporate prior information, and is conceptually simple. We also characterised the notion of sufficient, lossless, and optimal summaries in Section 2—distinctions that are important for developing compression algorithms and resolving misunderstandings, as discussed in Section 4.5.

We compared various methods on a benchmark problem (Section 5.1), the inference of parameters of a population genetics model (Section 5.2), and learning the parameters of a model for growing trees (Section 5.3). Minimising the EPE yields highly informative summaries—even for complex and multimodal posteriors—while achieving the long-standing goal of “finding methods which do not require a preliminary subjective feature selection stage” [27, p. 147]. But there is no free lunch: We instead have to choose a compression and density estimation architecture. Choosing appropriate architectures can improve performance, reduce the number of simulations required [20], and even allow summaries to generalise across datasets of different sizes as demonstrated in the benchmark and growing trees experiments.

Sequential methods can reduce the computational burden of likelihood-free inference [22, 24, 25], but we focused on learning summaries by simulating directly from the prior predictive distribution for two reasons: First, we wanted to isolate the effect of summary selection without introducing possible confounders. We omitted regression adjustment for ABC samples [54] for the same reason. Second, learning global summaries allows for one-shot inference because we do not need to retrain models for each example. Investigating the interaction between sequential methods and learning summaries could shed light on how different aspects of the data inform parameters in different regions of the parameter space, as illustrated in Fig. 3.

The summaries of the mixture density networks employed in Section 5 could have arbitrary scales which can be problematic for ABC. We standardised summaries after extraction to mitigate this problem, but more general metric learning approaches could further improve ABC with MDN-compressed summaries [55]. Investigating the impact of model misspecification on ABC is an active area of research [56], and comparing the robustness of different summary selection methods should be considered in future work.

Neural density estimation has become a powerful tool for likelihood-free inference, “but there is no uniformly best algorithm” [57, p. 1]. ABC remains a compelling approach because of its theoretical properties, and it can produce high-fidelity posteriors—especially when low-dimensional but rich summaries can be extracted from complex data.
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8 EPE and expected Kullback-Leibler divergence

The difference between the EPE given only the summaries $t$ and the EPE given the underlying data $z$ is

\[ H - \mathbb{E}[H \{ f(\theta | z) \}]_{z \sim p(z)} = \int dz \, d\theta \, p(z, \theta) \log f(\theta | z) - \int dt \, d\theta \, p(t, \theta) \log f(\theta | t). \]

Changing variables of integration to $z$ in the second term and combining integrals yields

\[ H - \mathbb{E}[H \{ f(\theta | z) \}]_{z \sim p(z)} = \int dz \, d\theta \, p(z, \theta) \log f(\theta | z) - \log f(\theta | t(z)). \]

Splitting the joint distribution $p(z, \theta)$ into conditionals $p(z) f(\theta | z)$ and combining the logarithms gives the expression in the main text:

\[ H - \mathbb{E}[H \{ f(\theta | z) \}]_{z \sim p(z)} = \int dz \, p(z) \int d\theta \, f(\theta | z) \log \left( \frac{f(\theta | z)}{f(\theta | t)} \right). \]

9 Proposition of sufficiency by Chen et al.

Chen et al. [22] made the following proposition (see p. 2); we have adapted the notation for consistency with the main text.

**Proposition 1** Let $\theta \sim \pi(\theta)$, $z \sim g(z | \theta)$, and $t \in T$ be a deterministic function. Then $t = t(z)$ is a sufficient statistic for $g(z | \theta)$ if and only if

\[ t = \arg\max_{t' \in T} I \{ \theta, t'(z) \}, \tag{15} \]

where $I \{ \cdot, \cdot \}$ denotes the mutual information between two random variables.

However, as discussed in Section 2, the existence of sufficient statistics is a property of the likelihood—not the approach used to compress the data. The statistic in Eq. (15) is sufficient if and only if the likelihood belongs to the exponential family. If the likelihood does not belong to the exponential family, the statistic is optimal in the sense that it minimises Eq. (2) with loss functional being the expected Kullback-Leibler divergence, as discussed in Section 3.

They subsequently argued that “the sufficiency of the learned statistics is insensitive to the choice of $\pi(\theta)$” (p. 4) and that the “approach differs from [other] methods as it is globally sufficient for all $\theta$” (p. 6). As demonstrated in Section 4.5, this assertion does not hold in general. But it is true if the likelihood belongs to the exponential family and $T$ includes the sufficient statistics. The proof proposed by Chen et al. [22] does not hold because it assumes the conclusion (p. 13).
10 Likelihood-based inference for the benchmark problem

We used the likelihood-based inference framework Stan [7] to draw samples from the posterior for the benchmark problem in Section 5.1. The algorithm uses the geometry of the posterior to efficiently draw samples from it. However, complex geometries make exploring the posterior difficult, and a change of variables can be an effective means to improve sampling. For the problem at hand, we made the change of variables \( \phi = \tanh \theta \) such that the likelihood becomes

\[
y_i \mid \phi \sim \frac{1}{2} \sum_{u \in \{-1,1\}} \text{Normal} \left( u \times \phi, 1 - \phi^2 \right)
\]

and we restricted \( 0 \leq \phi < 1 \) because the posterior is symmetric and exploring one mode is sufficient. The posterior is thus

\[
p(\phi \mid y) \propto \frac{1}{1-\phi^2} \times p \left( \theta = \tanh^{-1} \phi \right) \times \prod_{i=1}^{n} p\left(y_i \mid \phi\right),
\]

where the first term is the Jacobian accounting for the change of variables. We obtained samples of \( \theta \) by applying the inverse tanh transform and randomly reversing the sign with probability 0.5. We set the target acceptance probability to 0.99 to ensure that there are no divergent transitions which indicate numerical instabilities [7].
Table 1: *The quality of summaries has a significant impact on the fidelity of posteriors.* The table reports the negative log probability loss (NLP) and root mean integrated squared error (RMISE) for combinations of methods and experiments; reported errors are standard errors. Methods that are within one standard error of the best method are highlighted in bold. See Sections 5.1 to 5.3 for details on the benchmark, coalescent, and growing tree experiments, respectively.

| Method            | Benchmark |         | Coalescent |         | Growing tree |         |
|-------------------|-----------|---------|------------|---------|--------------|---------|
|                   | NLP       | RMISE   | NLP        | RMISE   |              | NLP     | RMISE   |
| Likelihood-based  | 1.05 ± 0.01 | 1.24 ± 0.02 | not applicable | −0.666 ± 0.028 | 0.165 ± 0.002 |
| MDN compression   | 1.05 ± 0.01 | 1.24 ± 0.02 | 3.601 ± 0.028 | 3.82 ± 0.03 | −0.730 ± 0.021 | 0.167 ± 0.002 |
| MDN               | 1.08 ± 0.02 | 1.24 ± 0.02 | 3.595 ± 0.028 | 3.82 ± 0.03 | −0.727 ± 0.021 | 0.167 ± 0.002 |
| Nonlinear regression | 1.43 ± 0.02 | 1.35 ± 0.01 | 3.604 ± 0.028 | 3.82 ± 0.03 | −0.702 ± 0.021 | 0.172 ± 0.002 |
| Linear regression | 1.32 ± 0.02 | 1.30 ± 0.02 | 3.677 ± 0.029 | 3.98 ± 0.03 | −0.685 ± 0.021 | 0.174 ± 0.002 |
| Minimum CPE       | 1.13 ± 0.02 | **1.20 ± 0.02** | 3.734 ± 0.033 | 3.99 ± 0.03 | **−0.700 ± 0.022** | 0.169 ± 0.002 |
| Expert summaries  | 1.12 ± 0.01 | 1.25 ± 0.02 | 3.685 ± 0.025 | 4.05 ± 0.03 | −0.579 ± 0.014 | 0.208 ± 0.002 |
| PLS               | 1.15 ± 0.02 | 1.26 ± 0.02 | 3.712 ± 0.024 | 4.05 ± 0.03 | −0.525 ± 0.013 | 0.225 ± 0.002 |
| Prior             | 1.44 ± 0.03 | 1.36 ± 0.01 | 4.621 ± 0.003 | 5.69 ± 0.03 | 0.696 ± 0.002 | 0.801 ± 0.006 |