Curve fitting, as opposed to a standard nonlinear fit, becomes relevant when a data set has a significant uncertainty in the direction of the independent variable (sometimes referred to as errors-in-variables models) or the set of model curves includes relations which predicts multiple values for the same value of the independent variable. In this case, the standard fitting approaches, such as a “chi-squared analysis” become unusable. In the context of Bayesian inference, this work shows that one can construct a general formalism for curve fitting which is applicable to a wide variety of data analysis problems and is not yet published elsewhere. In this Letter, a Bayesian approach to curve fitting is described and compared to almost all previous works which have given similar techniques.

Bayesian inference often proceeds via the application of Bayes theorem, $P(M|D) = P(D|M)P(M)/P(D)$, and the process of fitting models to data begins with the construction the conditional probability of the data given the model, $P(D|M)$ (this will be referred to this as the likelihood function) and specifying the prior probability distribution, $P(M)$ (the probability distribution for the data, $P(D)$, is often not needed). Since the RHS of Bayes’ theorem involves a product, there is an obvious potential for ambiguity: a multiplicative factor can be removed from the conditional probability and placed in the prior distribution without any modification to the final result.

It is assumed that the set of (possibly correlated) data points may be represented by a single normalizable probability density function $D(x_1, x_2, \ldots, x_N)$ over $N$ quantities of interest. As an example, in the case that one has $N$ uncorrelated one-dimensional data points which have normally distributed errors, then $D$ is a product of $N$ Gaussian distributions. In the case that these one-dimensional data points have correlations in the form of a multi-dimensional Gaussian (the formalism below does not require this assumption), then

$$D(x_1, x_2, \ldots, x_N) \propto \exp \left[ -\frac{1}{2}(x_i - \mu_i)\Sigma_{ij}^{-1}(x_j - \mu_j) \right]$$

where $\mu$ is the peak and $\Sigma$ is a covariance matrix. In some cases, the quantities of interest can be grouped together into n-tuples, so the quantities of interest are relabeled and the data probability density distribution is rewritten

$$D(x_{ij}) \equiv D(x_1, x_2, \ldots, x_n, x_{21}, x_{22}, \ldots, x_{2n}, \ldots, x_{N1}, x_{N2}, \ldots, x_{Nn}).$$

The probability distribution $D$ may not directly represent data, but may refer to the posterior distribution obtained from a previous inference, and the methods described below are essentially unchanged.

It will be useful to classify models according to the dimensionality of their outputs. (This dimensionality does not depend on the data, except that it is specified as a probability distribution as described above.) A “zero-dimensional” model, $M$, with $M$ parameters, $\{p\} \equiv p_1, p_2, \ldots, p_M$, is a model which produces a set of $N$ predictions for each of the $N$ quantities of interest, $\hat{x}_1 = M_1(\{p\})$, $\hat{x}_2 = M_2(\{p\})$, $\ldots$, $\hat{x}_N = M_N(\{p\})$. In this case, the conditional probability $P(D|M)$ is equal to $D(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N)$. This is the case for which one can employ a standard chi-squared analysis (in that case the quantities of interest are the “$y$” values and the “$x$” values simply provide an index for the data points which is irrelevant for the fit). The frequentist best-fit is the maximum of $D(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N)$ over the full model parameter space, and if $D$ is of the form of Eq. 1 then the standard error analysis applies.

A “one-dimensional” model produces a probability density function for each point in parameter space rather than a unique value for each quantity of interest, i.e. $M_1(x_1, \{p\})$, $M_2(x_2, \{p\})$, $\ldots$, $M_N(x_N, \{p\})$. In this case, the conditional probability is the $N$-dimensional integral

$$P(D|M) = \int \prod_{i=1}^{N} [M_i(x_i, \{p\})dx_i] D(x_1, x_2, \ldots, x_N).$$

As is typical in Bayesian inference, a prior distribution over the model parameters must be specified as a separate probability distribution, $P_{\text{prior}}(\{p\})$, and then the
posterior distribution for, e.g., $p_1$ is

$$P(\hat{p}_1) \propto \int \prod_{i=1}^{N} dp_i \ \delta (p_i - \hat{p}_1) \ P(D|\mathcal{M}) P_{\text{prior}}(\{p\}).$$

An example of a one-dimensional model is a zero-dimensional model which has a fixed Gaussian uncertainty, $\varepsilon$, in its predictions, $\hat{x}_i$, for all of the quantities of interest. Presuming the data points have only Gaussian correlations of the form in Eq. 1, then likelihood in Eq. 3 can be written in the form

$$P(D|\mathcal{M}) \propto \prod_{i=1}^{N} \left\{ \exp \left[ -\frac{1}{2} \left( x_i - \hat{x}_i \right)^2 / (2\varepsilon^2) \right] \right\} dx_i \times \exp \left[ -\frac{1}{2} \left( x_i - \mu_i \right) \Sigma^{-1}_{ij} (x_j - \mu_j) \right]$$

$$= A \exp \left[ -\frac{1}{2} (\hat{x}_i - \mu_i) \Sigma^{-1}_{ij} (x_j - \mu_j) \right],$$

where $\Sigma_{ij} = \Sigma_{ij} + \delta_{ij} \varepsilon_i^2$ and $A$ is a normalization constant. Since the final result is a single multivariate Gaussian, Bayesian inference using one-dimensional models can be represented by a Gaussian process. Eq. 5 derives the result given in Eq. 2.20 in Ref. [1]. The frequentist best-fit (i.e. the maximum of the likelihood function), in the case of a one-dimensional model, is the maximum of the RHS of Eq. 3 over the parameter space, a maximization which requires, in general, the evaluation an $N$-dimensional integral over each point. After using the $\delta$ function to perform one of the integrations, the computation of the posterior distribution in Eq. 4 is an $N+M-1$ dimensional integral (though there are still only $M$ model parameters). Joint posteriors for multiple model parameters can be handled with multiple $\delta$ functions as above.

A two-dimensional model generates two-dimensional probability distributions over pairs of quantities of interest. The conditional probability is

$$P(D|\mathcal{M}) \propto \int \prod_{i=1}^{N} \left\{ \exp \left[ -\frac{1}{2} \left( x_{i1} - \hat{x}_{i1} \right)^2 / (2\varepsilon_{i1}^2) \right] dx_{i1} \right\} \times \delta_{i1} \times \exp \left[ -\frac{1}{2} \left( x_{i2} - \hat{x}_{i2} \right) \Sigma^{-1}_{ij} (x_j - \mu_j) \right]$$

$$= A \prod_{i=1}^{N} \left\{ \exp \left[ -\frac{1}{2} (\hat{x}_{i1} - \mu_{i1}) \Sigma^{-1}_{ij} (x_j - \mu_j) \right] \right\},$$

which is a $2N$-dimensional integral. Note that the pair of variables $(x_{i1}, x_{i2})$ need not be the same as the pair $(x_{21}, x_{22})$ and heterogeneous two-dimensional data sets may be fit using Eq. 6. Generalizations to higher dimensions (or problems with mixed dimensionality) are easily obtained.

The discussion above does not exhaust all of the potential possibilities, as a model may generate a manifold embedded in some higher dimensional space. The simplest example is a one-dimensional model which generates a curve embedded in a two-dimensional data space for each point in parameter space. The likelihood function, in this case, is

$$P(D|\mathcal{M}) \propto \int c_i(\{p\}) \ \prod_{i=1}^{N} \left\{ \exp \left[ -\frac{1}{2} \left( x_{i1} - \hat{x}_{i1} \right)^2 / (2\varepsilon_{i1}^2) \right] dx_{i1} \right\} \times \delta_{i1} \times \exp \left[ -\frac{1}{2} (\hat{x}_{i2} - \mu_{i2}) \Sigma^{-1}_{ij} (x_j - \mu_j) \right]$$

$$= A \prod_{i=1}^{N} \left\{ \exp \left[ -\frac{1}{2} (\hat{x}_{i1} - \mu_{i1}) \Sigma^{-1}_{ij} (x_j - \mu_j) \right] \right\},$$

where $c_i$ is the $i$-th curve (one curve for each data point and $N$ total data points) which the model produces given the parameter set $\{p\}$, $\lambda_i$ specifies the line element along the $i$-th curve, $g_{jk}$ represents the $i$-th metric for the line integral, $M_i(\lambda_i)$ is the probability distribution along the $i$-th curve which is specified by the model, and $\mathcal{D}(\{x_{i1}(\lambda_i)\})$ is the probability given by the data, evaluated at the point $\lambda_i$ on curve $c_i$. Indices $j$ and $k$ take values 1 and 2 and are summed over since they are repeated and generalizations to larger than data spaces with larger than two dimensions are straightforward.

As might be expected from the discussion above, this is an $N$-dimensional integral. In order to form posterior distributions from this conditional probability one must also perform a sum over all possible curves allowed by the model. In physical problems, one typically parameterizes the curve with a finite number of parameters and then posterior distributions are obtained by performing the associated integral as in Eq. 4 above.

Note that, since the expression above employs $x(\lambda)$ and $y(\lambda)$ but not $y(x)$ or $x(y)$, there is no requirement that the curves are functions. The curves need not be continuous (the functions $x(\lambda)$ and $y(\lambda)$ need not be continuous or differentiable in order for the line integral to have meaning). This means that model curves which “go through” the data multiple times carry more weight, unless the model (or prior distribution) disfavors such a scenario. Models which parameterize their predicted curves with a finite number of parameters often disfavor arbitrarily complicated curves. Also, models may vary the weight they assign to curves with longer lengths by ensuring that the weight, $M_i(\lambda_i)$, is proportional to $\ell_i^{-\alpha}$ given a finite curve length $\ell$ and some number $\alpha > 1$.

The surprising aspect of curve fitting is the appearance of the metric, $g_{jk}$, for each data point. In the simple case where $g_{jk} = \delta_{jk}$, the integrand contains the usual line element used to compute arc length. One intuitive way to see the metric ambiguity, in the $N = 1$ and $n = 2$ case (a fit of one data point over a two-dimensional space with a one-dimensional model), is to imagine that $x_{11}$ and $x_{12}$ have different units. In that case, the line integral appears nonsensical because the units cannot properly cancel under the square root. The line integral is invariant under reparameterizations of the curve but not under an arbitrary rescaling of the coordinates. An alternative way to see that the metric required is to note that the model curve may also be specified by a $M = \delta (x_2 - q(x_1, x_2))$ and the transforming this form to one similar to the one above requires a derivative $|\partial q / \partial x_1|$ which contains the ambiguity represented by the metric. Finally, the appearance of the metric is not solely mathematical. For
example, the process of fitting a theoretical curve to experimental measurement of a particle’s location at several points (with some uncertainty in the coordinate directions), without any other additional information, is possibly modified by black holes which have traveled near the particle of interest and modified the nature of spacetime near the trajectory.

The line elements, denoted \{\lambda\}, are nuisance parameters which must be integrated over. They also have prior distributions, which must be specified to complete the inference. The problem of Bayesian inference from this likelihood results in three possibilities: (i) the model may specify what metrics ought to be used (leaving the prior unspecified), (ii) the model may leave the metrics unspecified and then the choice of metric is also a prior choice, and (iii) the metric may be unnecessary or trivial because of some special feature of the model (e.g. if the quantities \(x_{ij}\) have the same units for all \(j\)). Options (i) and (ii) are related because of the product of the likelihood and prior is unchanged when multiplicative factors are moved between the two. Without some additional simplification, our model now effectively has \(N + M\) parameters, the \(M\) quantities \(\{p\}\) and the \(N\) line elements \(\{\lambda\}\).

One might suggest that one can obtain the likelihood for the curve through a limiting procedure applied to the space in which it is embedded, and thus avoid the ambiguity from the metric. However, the limiting procedure is not unique. This is the Borel-Kolmogorov paradox [2, 3], and the specification of the metric in Eq. 7 avoids this paradox.

The conditional probability in Eq. 7 reproduces a traditional chi-squared fit in the case that the data has no uncertainty in one direction. For example, if

\[
D(x_{11}, x_{12}, x_{21}, x_{22}, \ldots, x_{N1}, x_{N2}) \\
\propto \prod_i \exp \left( -\frac{\sum_{j=1}^{N} (x_{ij} - \mu_i)^2}{2\sigma_i^2} \right) \delta(x_{2i} - \eta_i) \ , \quad (8)
\]

then one can choose \(g_{jk} = \delta_{jk}\) for all \(i\), \(\lambda_i = x_{2i}(x_{1i})\), and use the delta functions in \(D\) to do the line integrals. The factor \(M(\lambda)\) only serves to reweight the data points and can be removed, finally leading to the conditional probability for a typical chi-squared fit.

A frequentist equivalent could select the model which maximizes \(P(D|M)\) over the parameter space. In the case of curve fitting (Eq. 7) this optimization problem is itself difficult, and the subject of algorithms designed to perform this optimization (e.g. Ref. [4]). In our Bayesian approach where the integrals are often computable, in principle, using Monte Carlo methods, but specific problems may result in functions which are difficult to integrate.

A simpler alternative approach to Eq. 7 is to replace each line integral in with a maximization. The alternative likelihood of a curve labeled \(c\) is

\[
\mathcal{L}_{alt}(c) = \prod_i^{N} \text{Max}_{\lambda_i} [D_i(x_1, x_2, \ldots, x_n)M(\lambda_i), c] \ , \quad (9)
\]

where the \text{Max} function picks out the point along the curve \(c\) which has the largest value of the product \(DM(\lambda)\). However, the replacement of the line integral by a maximization forces one to give up on coherence since some possible combinations of model parameters and values for the parameters of interest are arbitrarily removed from the posterior distribution [5].

Eq. 7 presumes that the model predicts the shape of the curve with zero uncertainty. This may not be the case, and the uncertainty may increase the dimensionality of the problem leading to fitting a surface (or manifold) to data rather than just a curve. When the model generates a manifold, the formalism above can be easily generalized, except that the metric on the manifold requires a prior specification corresponding to the dimensionality of the manifold. For example, a model which generates a two-dimensional surface gives a surface integral over the data and requires a prior distribution with two additional degrees of freedom corresponding to the two dimensions in the surface.

The uncertainty in the curve \(\lambda_i\), parameterized by some quantity \(\eta_i\) may also lie in either the \(x_{i1}\) or \(x_{i2}\) directions. In this case, the model must specify the probability distribution for the set of possible curves and how to sum over this set. When the model makes this specification, it is effectively specifying the relationship between \((\lambda_i, \eta_i)\) and \((x_{i1}, x_{i2})\). Thus any integration over \(\lambda_i\) and
\( \eta \) can be transformed to an integration over \( x_{11} \) and \( x_{11} \) and the conditional probability reduces to the form given in Eq. 6.

Similar curve fitting problems have been the subject of work in frequentist data analysis, leading to several different approaches, much of it focused on the case when the data points are nearly normally distributed in both the \( x_{11} \) and \( x_{22} \) directions and the curve to fit is nearly linear. In this case, one can use traditional least squares in either the \( x \)- or \( y \)-direction, total least squares, orthogonal least squares (a special case of total least squares), or geometric mean (or reduced major axis) regression [7]. Traditional least-squares in the \( y \)-direction, for example, corresponds to the choice \( g_{jk} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \), \( \lambda = y \), and ignores the variation of the data in the \( x \) direction. Orthogonal least squares does not simply map on to Eq. 7, but corresponds to using a rotation matrix for the metric with an orientation dictated by the slope of the curve near each data point and then ignores the data variation orthogonal to the rotation matrix. Ref. [8] compares related methods for a particular class of problems from a frequentist perspective. None of these methods, however, applies to the most general case when the curves are highly nonlinear.

There are previous works which cover curve fitting in the Bayesian perspective, most again on Gaussian distributed uncertainties where the variance in the two coordinate directions naturally provides a scale which help define the metric. Ref. [9] describes line fitting for errors-in-variables models and describes the conditions under which the solution is not possible due to matrix singularities. (The likelihood in Eq. 7 will similarly exhibit difficulties if the metric is singular. Ref. [10] performs a fit assuming a nearly linear curve, and uses the approximation that the line integral over the probability distribution from the data is approximately Gaussian. Ref. [11] also analyzes the nearly linear case with Gaussian uncertainties in the data. Ref. [11] considers the an additional uncertainty in the \( y \) direction and obtains a modification similar to the result in Eq. 5. None of these works describes the general result in Eq. 7 above. Ref. [12] describes a complementary geometric method to fitting lower-dimensional models to data in the context of Bayesian inference. The discussion above, however, is unique in its identification of the ambiguity from the metric and the observation that the metric choice may need to be part of the prior.

Ref. [6] describes the Bayesian generalization of orthogonal least squares, and fits a sample Gaussian data set to a line to demonstrate the approach (see figure 9 in Ref. [6]). In figure 1, the same data set is shown including an analysis with the likelihood in Eq. 7. A nearly indistinguishable result is obtained, demonstrating that our formalism works with a simple problem. A more physical example is in Ref. [13] where theoretical neutron star cooling curves are compared with data. In this case, the use of Eq. 7 is required because of large uncertainties in the age observations. There is no clear model guidance on the metric so a simple choice is made.

A more difficult fitting problem which demonstrates the method and cannot be easily solved from the method in Ref. [6] is that shown in figure 2 which is fit to a model curve \( r = a \theta \) which could not be easily performed using traditional regression techniques. The parabolic contours give 68% contours for the 10 data points, the density plot shows the posterior of the fit with trivial metric for \( \theta > 1.6 \), and the inset compares the posterior distribution for the parameter \( a \) using either the trivial metric (solid line) or modified metric (dashed line). The prior probability distributions for \( a \) and \( \lambda = \theta \) are taken to be uniform for both metrics.

FIG. 2: A fit of sample data to a one parameter model \( r = a \theta \) which could not be easily performed using traditional regression techniques. The parabolic contours give 68% contours for the 10 data points, the density plot shows the posterior of the fit with trivial metric for \( \theta > 1.6 \), and the inset compares the posterior distribution for the parameter \( a \) using either the trivial metric (solid line) or modified metric (dashed line). The prior probability distributions for \( a \) and \( \lambda = \theta \) are taken to be uniform for both metrics.

In summary, a new Bayesian approach to curve fitting has been presented which applies to a wide variety of problems and suffers from no ambiguity beyond the proper specification of the prior probability. It gives
the correct result in the limiting case of a straight line fit. Our approach generalizes to higher dimensional cases where the model produces a manifold embedded in a higher-dimensional space occupied by the data. From the Bayesian perspective, much of the frequentist literature on this problem attempting to optimize the choice of frequentist method for the problem at hand is equivalent to trying to optimize the choice of prior distribution. Thus, one expects that objective Bayesian priors such as the Jeffrey’s prior could be applied to this problem, and this possibility is left to future work.

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