Root mean square error (RMSE) or mean absolute error (MAE): when to use them or not

Timothy O. Hodson¹

¹U.S. Geological Survey Central Midwest Water Science Center, Urbana, IL **Correspondence:** Timothy O. Hodson (thodson@usgs.gov)

Laplacian errors. When errors deviate from these distributions, other metrics are superior.

Abstract. The root mean squared error (RMSE) and mean absolute error (MAE) are widely used metrics for evaluating models. Yet, there remains enduring confusion over their use, such that a standard practice is to present both, leaving it to the reader to decide which is more relevant. In a recent reprise to the two-century-long debate over their use, Willmott and Matsuura (2005) and Chai and Draxler (2014) give arguments for favoring one metric or the other. But this comparison can present a false dichotomy. Neither metric is inherently better: RMSE is optimal for normal (Gaussian) errors, and MAE is optimal for

Introduction

The root mean squared error (RMSE) and mean absolute error (MAE) are two standard metrics used in model evaluation. For a sample of n observations $y(y_i, i = 1, 2, ..., n)$, and n corresponding model predictions \hat{y} the MAE and RMSE are

10 RMSE =
$$\sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$
 (1)

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i|.$$
(2)

As its name implies, the RMSE is the square root of the mean squared error (MSE). Taking the root does not affect the relative ranks of models, but it yields a metric with the same units as y, which conveniently represents the typical or "standard" error for normally distributed errors. The MSE and MAE are averaged forms of the L2-norm and L1-norm, which are the Euclidean and Manhattan distance, respectively.

In what have become two classic papers in the geoscientific modeling literature, Willmott and Matsuura (2005, MAE) and Chai and Draxler (2014, RMSE) discuss whether RMSE or MAE is superior. In their introduction, Chai and Draxler (2014) state:

"The RMSE has been used as a standard statistical metric to measure model performance in meteorology, air quality, and climate research studies. The MAE is another useful measure widely used in model evaluation. While they have both been used to assess model performance for many years, there is no consensus on the most appropriate metric for models errors."

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The statement may have accurately characterized the application in geosciences but not in statistics. Among statisticians, the answer was common knowledge, at least to the extent that there can be no consensus. Different types of models have

different error distributions and so necessitate different error metrics. In fact, the debate over squared versus absolute error terms had emerged, was subsequently forgotten, and reemerged over the preceding two centuries (Boscovich, 1757; Gauss, 1816; Laplace, 1818; Eddington, 1914; Fisher, 1920), with history given by (Stigler, 1973, 1984), making it one of the oldest questions in statistics.

It is unclear exactly when this "no-solution solution" became common knowledge, in part, because contemporary authors rarely cite its sources. While reviewing the literature, I found proofs in several reference works, including the venerable Press et al. (1992, p. 701), but no references to the primary literature.

As this review will show, the choice of error metric should conform with the expected probability distribution of the errors; otherwise, any inference will be biased. The choice of error metric is, therefore, fundamental in determining what scientists learn from their observations and models. This paper reviews the basic justification for choosing between RMSE or MAE, then

35 discusses several alternatives better suited for the complex error distributions that are encountered in practice. The literature on this topic is vast, and I try to emphasize classic papers and textbooks from the statistical literature. To make that discussion more concrete, I include several examples from hydrology and rainfall-runoff modeling, though none of the techniques are exclusive to that field. The discussion is primarily written for Earth scientists who use RMSE or MAE but have little-to-no awareness of formal likelihood methods.

40 2 The naive (frequentist) basis

Willmott and Matsuura (2005) and Chai and Draxler (2014) present several arguments both for and against RMSE and MAE. I will not review them here; instead I will describe the theoretical justification for either metric. Both RMSE and MAE are derived from the laws of probability, which themselves are derived from the laws of logic (Jaynes, 2003); thus, there are logical reasons for choosing one metric over the other.

45 Like all inference problems, the justification begins with Bayes' theorem,

where y is some set of observations, θ are the model parameters, and $p(\theta|y)$ is the probability of θ given y. In words, Bayes' theorem represents the logical way of using observations to update our understanding of the world. The numerator of the right-hand side contains two terms: the prior, representing our state of knowledge before observing y; and the likelihood, representing

50 what was learned by observing y. The left-hand side, known as the posterior, represents our updated state of knowledge after the observation. Given a set of observations y, the denominator of the right-hand side is constant, so, for convenience, Bayes' theorem is often rewritten as the proportion between the posterior and the product of the likelihood with the prior,

$$p(\theta|y) \propto p(y|\theta)p(\theta).$$
 (4)

In the absence of any prior information the prior distribution $p(\theta)$ is "flat" or constant, such that the posterior is simply 55 proportional to the likelihood,

$$p(\theta|y) \propto p(y|\theta).$$
 (5)

This relation provides the basis for "frequentist" statistics, first recognized by Bernoulli (1713) and later popularized by Karl Pearson, Ronald Fisher, and others. Criticisms of frequentism aside (see Clayton, 2021, for summary), the recognition that without strong prior information the simpler problem of deduction (using a model to predict data) could be substituted for

60 the harder problem of induction (using data to predict a model) would determine the course of 20th-century science. The substitution is expressed formally as

$$\mathcal{L}(\theta|y) = p(y|\theta),\tag{6}$$

where \mathcal{L} is used to represent the likelihood so that it is not confused with the posterior probability distribution $p(\theta|y)$. Absent any strong prior information, one can apply this substitution to infer the most likely model parameters θ given some data y. Because probability theory conforms with logic, the logical choice is to select, or at least prefer whatever model maximizes the likelihood function. This basic argument provides the basis for maximum likelihood estimation (MLE, Fisher, 1922), which are a class of methods for selecting the model θ having the greatest likelihood of having generated the data; formally,

$$\theta_{MLE} = \operatorname{argmax}_{\theta}(\mathcal{L}(\theta|y)),\tag{7}$$

where $\hat{\theta}_{MLE}$ represents the MLE estimate of θ . The justification of MLE leads directly to the justification of RMSE and MAE, 70 because under certain conditions the MSE and MAE are inversely proportional to the log likelihood. That is to say, the model that minimizes the appropriate metric is also the more likely, but understanding exactly why this is so requires a bit more explanation.

3 The normal case

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First, the case of normally distributed (Gaussian) errors. Consider a normally distributed variable y and some corresponding set 75 of normally distributed model predictions \hat{y} . The model error is, therefore, the difference between two normal distributions. If y and \hat{y} are independent, the error distribution is guaranteed to be normal. Such a model provides no information, however, and for a model to be useful, \hat{y} and y should be dependent. Although the difference between two dependent normal distributions is not guaranteed to be normal, it will often be so (Kale, 1970). Thus, we say that normally distributed variables will tend to produce normally distributed errors. As a starting point, assume the prediction errors are normal and independent and 80 identically distributed (*iid*). Ways of relaxing these assumptions are introduced in the next sections, but they provide a strong

80 identically distributed (*iid*). Ways of relaxing these assumptions are introduced in the next sections, but they provide a strong foundation, evident by the popularity of ordinary least squares. Our goal, then, is to identify the model f() with normal *iid* errors that is most likely given the data y, where f() has inputs x and parameters θ , written as $f(x, \theta)$. The output of $f(x, \theta)$ is the model prediction \hat{y} , which represents the conditional mean of y given θ and x,

To find the most likely model, we begin with the likelihood given by the normal distribution,

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$$\mathcal{L}(\mu,\sigma|y) = \frac{1}{\sqrt{2\pi\sigma^2}} \prod_{i=1}^{n} \exp\left[-\frac{(y_i - \mu)^2}{2\sigma^2}\right],$$
 (8)

where Π is the product of the terms, μ is the population mean and σ is the standard deviation. Next, $f(\theta, x)$ is substituted for μ , replacing the population mean with the conditional mean,

$$\mathcal{L}(\theta,\sigma|y,x) = \frac{1}{\sqrt{2\pi\sigma^2}} \prod_{i=1}^{n} \exp\left[-\frac{(y_i - f(\theta,x_i))^2}{2\sigma^2}\right].$$
(9)

A convenient practice is to take the logarithm of the likelihood, thereby converting the products to sums

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$$\log \mathcal{L} = -n\log\sigma - \frac{n}{2}\log(2\pi) - \frac{1}{2\sigma^2}\sum_{i=1}^n (y_i - f(\theta, x_i))^2,$$
 (10)

logging does not change the location of maximum, so it does not change the MLE estimate. From equation 10, it can be seen that maximizing the log-likelihood for the parameters θ is equivalent to minimizing the sum

$$\sum_{i=1}^{n} (y - f(\theta, x_i))^2, \tag{11}$$

which is the L2-norm. Dividing by n also has no effect on the location of the maximum of the log-likelihood and yields the

MSE. Thus, for normal *iid* errors, the model that minimizes the MSE (or the L2-norm) is the most likely model, all other things 95 being equal. Although beyond our scope, information criteria, Bayesian methods, and cross validation are all techniques for dealing with situations where all other things are not equal and are closely related to topics discussed in this review.

4 The Laplace case

Now consider an exponentially distributed random variable; a concrete example being daily precipitation, which is often approximately exponential in distribution. If both model predictions and observations are *iid* exponential random variables, 100 then the model error will have a Laplace distribution (sometimes called a double exponential distribution). Like the normal case, such a model is not useful, so instead we focus on models for which predictions and observations are dependent. Such a model is not guaranteed to have Laplacian errors; nevertheless, its errors will tend to exhibit strong positive kurtosis, so we say it tends toward Laplacian-like error.

105 Assuming the Laplace distribution better represents the error than the normal, than we should prefer the model maximizing the Laplacian likelihood function,

$$\mathcal{L}(\theta, b|y, x) = \frac{1}{2b} \exp\left[-\frac{|y - f(\theta, x_i)|}{b}\right],\tag{12}$$

where b is a parameter of the distribution. Here we use the same substitution as in equation 9 to convert from the standard Laplace distribution to a Laplacian-error distribution. The log-likelihood is then

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$$\log \mathcal{L} = -n\log(2b) - \frac{1}{b}\sum_{i=1}^{n} |y_i - f(\theta, x_i)|,$$
 (13)

and repeating the argument from the normal case, maximizing the log-likelihood for θ is equivalent to minimizing the sum

$$\sum_{i=1}^{n} |y - f(\theta, x_i)|,\tag{14}$$

which is the L1-norm. Dividing the L1-norm by n yields the MAE. Thus, for Laplacian errors, the model that minimizes the MAE (or the L1-norm) also maximizes the likelihood.

115 5 Other options

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To summarize the previous two sections: for normal errors, minimizing either MSE or RMSE yields the most likely model; whereas for Laplacian errors, minimizing MAE yields the most likely model. Normally distributed variables tend to produce normally distributed errors, and exponentially distributed variables tend to produce Laplacian-like errors, so RMSE and MAE are reasonable first choices for each case, respectively. Technically both also assume the errors are *iid*, and, for many interesting problems, errors are neither perfectly normal, nor Laplacian, nor *iid*. In these cases, there are essentially four options, all somewhat interrelated and often used in conjunction.

5.1 Refine the model structure

The first option is to refine the structure of the model; in other words, make the model more physically realistic. While this option is the most important for the advancement of science, it is not relevant to the choice of error metric, so I will not

125 discuss it further, other than to note that likelihoods can also be used to evaluate model structure: first, determine the maximum likelihood for each candidate model structure, then select (or prefer) the most likely among these candidates (e.g., Burnham and Anderson, 2001). The preceding derivations were formulated in terms of maximizing the likelihood by way of adjusting the model parameters θ , but more generally, the likelihood can be used to refine the entire model—both its parameters and structure.

130 5.2 Transformation

The second option is to transform the data to a Laplace or, more commonly, normal distribution, then minimizing the RMSE or MAE of the transformed data will yield the most likely model. For example, the streamflow distribution of a perennial stream is approximately lognormal. Logging a lognormal variable yields a normal one, so in log space, the error is the difference between two normal distributions, which will also tend to be normal. If the errors can be made normal by transformation, then

135 minimizing the MSE of the transformed variable will yield the most likely model. Many statistical methods assume normality, and the general name for transforming a non-normal variable into a normal one is known as a Box-Cox transformation (Box and Cox, 1964). Transformations can make results harder to interpret, but this is usually an acceptable trade-off for better inference.

5.3 Robust inference

140 The third option is to use "robust" methods of inference. The term "robust" signifies that a technique is less sensitive to violations of its assumptions; typically, meaning they are less sensitive to extreme outliers. To achieve this, robust techniques replace the Gaussian likelihood with one with thicker-tails, such as the Laplace or the Student's-t, which reintroduces the choice between RMSE and MAE, as MAE corresponds to the Laplace likelihood.

While Fisher (1920) demonstrated that minimizing the squared error was theoretically optimal for normal errors, he permitted Eddington to add a footnote that in practice, better results were often achieved by minimizing the absolute error, because in practice, observations include some outliers that deviate from the normal distribution (Stigler, 1973). For this reason, minimizing the MAE has come to be known as a "robust" form of MLE, as in "robust regression" (e.g., Murphy, 2012, section 7.4). Tukey, in particular, was seminal in developing and exploring robust methods, such as in Tukey (1960) and his contributions to the field are documented by Huber (2002).

150 In this discourse, Willmott et al. (2009) recognize robustness as an important advantage of MAE, though Chai and Draxler (2014) never directly acknowledge this point and instead advocate for "throwing out" outliers. Neither option is ideal. Either can yield reasonable results for minor deviations from the normal, but their performance degrades as the deviation grows.

Since Tukey's work, more robust alternatives have emerged, including the median absolute deviation or MAD,

$$MAD = b \operatorname{median}_{i=1}^{n} |\hat{y}_{i} - \operatorname{median}(y)|, \tag{15}$$

- 155 where typically b = 1.483 to reproduce the standard deviation in the case of the normal distribution (denoted as MAD_{σ}). Although MAD is less theoretically grounded, empirical evidence indicates it is more robust than MAE. MAD was first promoted by Hampel (1974), who attributed it to Gauss, and later by Huber (1981), and more recently by Gelman et al. (2020). One drawback is its relative inefficiency for normal distributions (Rousseeuw and Croux, 1993), but advocates of MAD counter that RMSE is as inefficient (or more) for error distributions that deviate from the normal, so MAD remains a popular choice.
- 160 In addition to being "robust," MAD and MAE also preserve scale, unlike the formal likelihood-based approach discussed next. Unless combined with a transformation, scale-preserving error metrics have the same units as the data, such that their magnitude roughly corresponds to the magnitude of the typical error. While MAD and MAE are easy to interpret and implement, they are somewhat limited in scope in that they are only appropriate for "contaminated" distributions— mixtures of normal or Laplace distributions with a common midpoint, which, by implication, are also symmetric.
- More complicated error distributions are frequently encountered in practice. For example, errors in rainfall-runoff models are typically heteroscedastic. Log transforming the data can correct this for positive streamflows values, but the log is undefined when streamflow is zero or negative. Simple work arounds, such as setting zeros to a small positive value, may be satisfactory when zero and near-zero values are relatively rare but blow up as those values become more frequent. Recall that in log space, errors are proportional, so the difference between 0.001 and 1 is the same as that between 1 and 1000.

170 5.4 Likelihood-based inference

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The final option, likelihood-based inference, is the most versatile and subsumes the others in that each can be incorporated within its framework. Its main drawback is interpretative. The absolute value of the likelihood is meaningless, unlike RMSE or MAE, which measure the typical error. Their relative values are meaningful, however, in that the likelihood ratio represents the evidence for one model relative to another. For an accessible introduction to likelihood-based model selection, the reader is referred to Edwards (1992) and Burnham and Anderson (2001).

Metrics like RMSE and MAE are sometimes referred to as "informal" likelihoods because, in certain circumstances, they yield results equivalent to those obtained by the "formal" likelihood (e.g., Smith et al., 2008). Recall that the model that minimizes the RMSE also maximizes the likelihood, if the errors are normal and *iid* (11). Informal likelihoods share some of the flexibility of formal ones, while preserving scale (commonly as real or percentage error). However, they have two notable

- 180 drawbacks. Formal likelihoods are necessary when combining different distributions into one likelihood or when comparing among different error distributions (e.g., normal versus Laplace; Burnham and Anderson, 2001). Furthermore, because informal likelihoods obscure their probabilistic origins, practitioners are frequently unaware of them and, as a consequence, use them incorrectly.
- For rainfall-runoff modeling, examples of the formal likelihood-based approach include Schoups and Vrugt (2010); Smith et al. (2010, 2015). Schoups and Vrugt (2010) create a single flexible likelihood function with several parameters that can be adjusted to fit a range of complex error distributions; whereas, Smith et al. (2015) show the process of building complex likelihoods from combinations of simpler elements. Smith et al. (2015) focus on several variants of the zero-inflated normal distribution, which, in essence, inserts a normal likelihood within a binomial one. Additional components can be added to deal with heteroscedasticity and serial dependence of errors, which are typical in rainfall-runoff models. For example, in the
- 190 zero-inflated lognormal, a binomial component handles zeros values, while a log transformation handles heteroscedasticity in the positive values.

6 Why not use both RMSE and MAE?

Chai and Draxler (2014) argue for RMSE as the optimal metric for normal errors, refuting the idea that MAE should be used exclusively. They do not contend RMSE is inherently superior and instead advocate that a combination of metrics, including
both RMSE and MAE, should be used to evaluate model performance. Many models are multi-faceted, so there is an inherent need for multi-faceted evaluation, but it can be problematic if approached without considerable thought.

RMSE and MAE are not independent, so if both are presented, how should we weigh their relative importance when evaluating a model? Assuming no prior information, the logical approach is to weigh them by their likelihoods. According to the law of likelihoods, the evidence for one hypothesis versus another corresponds to the ratio of their likelihoods (Edwards, 1992,

200 p. 30). Extending this further, either metric can be weighted based on its relative likelihood (Burnham and Anderson, 2001).

If the evidence strongly supports one over the other, presenting both metrics is unnecessary and potentially confusing. If their evidence is similar, it may be appropriate to present a weighted average or present both metrics along with their weights (Burnham and Anderson, 2001). When averaging informal likelihoods to estimate the typical error, an additional adjustment must be made for differences in their scale, as demonstrated with MAD. Priors can be incorporated as well, though this is a

205 more advanced topic.

> Although the likelihood can provide an objective measure of model performance, we are often concerned with multiple facets of a model, such that any one performance metric is insufficient. A common solution is to define and compute several metrics, each chosen to characterize a different aspect of the model's performance. For example, in rainfall-runoff modeling a modeler may compute the error in flow volume (the model bias), as well the errors at a range of flow quantiles.

- 210 When evaluating these metrics, there is a tendency to combine them into an overall score, but such scores are not inherently meaningful, at least in a maximum-likelihood sense. A better, or at least safer, approach is to focus on a single objective function, like MSE for normally distributed errors. For the normal case, minimizing the MSE (or normal log likelihood) is optimal, because it minimizes the information loss (as information and negative log likelihood are equivalent). Typically we want to know more about a model than its general performance, however, such as how well it performs at specific tasks.
- 215 For that reason, we may choose to compute ancillary metrics, or, more formally, decompose the likelihood into components representing specific aspects of a model's performance (e.g., Hodson et al., 2021). It is also possible to combine several metrics into a valid likelihood, known as a mixture distribution, like the zero-inflated lognormal. In that case, the compound metric is valid, because the components are normalized to the same scale and do not contain duplicate information.

This review has focused primarly on how probability theory can answer the question "which model is better?", thereby guiding the task of model selection. But this task is equivalent to asking "how accurate is my model?", then comparing 220 competing models, and selecting the most accurate. That first step—quantifying the uncertainty in a model— is important in its own right, especially if we base decisions on predictions from our models. Just as the Gaussian likelihood provides the theoretical basis for using RMSE to quantify model uncertainty when errors are normally distributed, more generally, other likelihood functions are used to evaluate model accuracy and confidence intervals for other error distributions.

Conclusions 225 7

Probability theory provides a logical answer to the choice between RMSE and MAE. Either metric is optimal in its correct application; though in practice, neither may be sufficient. For these cases, refining the model, transforming the data, using robust statistics, or constructing a better likelihood can yield better results. Arguably the latter is most versatile, though there are pragmatic reasons for preferring the others.

- Returning to the discourse over MAE and RMSE. Chai and Draxler (2014) were correct that RMSE is optimal for normally 230 distributed errors, though they seem to suggest, wrongly, that MAE only applies to uniformly distributed errors. Though Willmott and Matsuura (2005) and Willmott et al. (2009) were correct that MAE is more robust, there are better alternatives. Most importantly, neither side provides the theoretical justification behind either metric, nor do they adequately introduce the extensive literature on this topic. Hopefully, this paper fills that gap by explaining why and when these metrics work, and exposing readers to several alternatives when they don't. 235

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