A generalized AIC for models with singularities and boundaries

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Abstract: The Akaike information criterion (AIC) is a common tool for model selection. It is frequently used in violation of regularity conditions at parameter space singularities and boundaries. The expected AIC is generally not asymptotically equivalent to its target at singularities and boundaries, and convergence to the target at nearby parameter points may be slow. We develop a generalized AIC for candidate models with or without singularities and boundaries. We show that the expectation of this generalized form converges everywhere in the parameter space, and its convergence can be faster than that of the AIC. We illustrate the generalized AIC on example models from phylogenomics, showing that it can outperform the AIC and gives rise to an interpolated effective number of model parameters, which can differ substantially from the number of parameters near singularities and boundaries. We outline methods for estimating the often unknown generating parameter and bias correction term of the generalized AIC.

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1. Introduction

Information criteria, such as the AIC [1], are often used to select a candidate model from several, or for weighting such models [2, 3]. Standard derivations of these information criteria require regularity conditions, which can be violated
when the generating parameter is a singularity or boundary of the parameter space. At such points, application of standard information criteria may not be theoretically justified and can perform poorly. Although violation of such conditions is not uncommon in practice, such as with latent class analysis [4, 5], or more general mixture models or models with constrained parameters [6], robustness to model violations is seldom raised. In particular, the AIC is often used without consideration of the effect of parameter space geometry on its behaviour.

Given a candidate model satisfying regularity conditions with parameter space $\Theta_0$, the AIC for the sum $Z_n$ of $n$ i.i.d. random observations $Z_i$ and maximum likelihood estimate $\hat{\theta}_n \in \Theta_0$ is

$$
\text{AIC} = -2 \log L \left( \hat{\theta}_n | Z_n \right) + 2 \dim (\Theta_0).
$$

The AIC’s bias correction term, $2 \dim \Theta_0$, is twice the number of parameters of $\Theta_0$. However, this correction can be inaccurate or ambiguous when regularity conditions are violated, such as for models with singularities and boundaries, where the notion of dimension is more nuanced. Away from singularities and boundaries, the expected value of the AIC at generating parameter $\theta_0$ is asymptotically equivalent to a quantity $\Delta_n (\Theta_0, \theta_0)$, called the target. The target is related to the Kullback-Leibler divergence of the candidate model distribution at $\hat{\theta}_n$ from the generating model distribution at $\theta_0$. (See Equation (1) for a precise definition.) By choosing a model with minimal AIC, a practitioner seeks one that minimizes information loss.

When $\theta_0$ is a singularity or boundary of $\Theta_0$, however, the bias correction $2 \dim \Theta_0$ is not generally asymptotically equivalent to its target. While the likelihood term of the AIC is retained in the generalized AIC (AICg) developed here, for a parameter space with singularities or boundaries, the AIC bias correction can be modified to ensure the expected AICg is asymptotically equivalent to its target. Informally, if singularities or boundaries are present, the parameter space may “behave” as if there is a different number of parameters than the naive count gives. This effective number of parameters $k_e$ need not be an integer, and can be smaller or larger than the number of parameters $k = \dim (\Theta_0)$.

A non-integral $k_e$, such as that appearing in the AICg bias correction, is not a new concept. It was introduced by Moody [7] in the context of non-linear learning systems and appears in the deviance information criterion (DIC) of Spiegelhalter et al. [8]. The AICg treats $k_e$ in a different way to ensure asymptotic equivalence of the expected AICg to its target.

In the AICg, $k_e$ is a function of $\theta_0$, and thus can vary across $\Theta_0$. Since in practice $\theta_0$ is typically unknown, methods are outlined here to estimate the AICg, the simplest of which is to replace $\theta_0$ with $\hat{\theta}_n$.

For a model with $k$ parameters, the expected AIC underestimates its target when $k < k_e$, and overestimates when $k > k_e$. We derive the AICg explicitly for models from phylogenomics in Section 2.3, including one where $k_e < k$ and one where $k > k_e$. 
The definition of regular models varies considerably in the literature, though a key part of the definition is always that Fisher information matrices are non-
singular \cite{9, 10}. (See also the assumptions of Theorem 16.7 of van der Vaart \cite{11}).
Watanabe defines singular models as those not having a one-to-one map between
parameters and probability distributions and/or not having Fisher information
matrices that are always positive definite. Models with singularities in their
parameter spaces may not be singular according to this definition. Thus, while
the widely applicable information criterion (WAIC) \cite{12} generalizes the AIC to
singular models in the sense of Watanabe \cite{9}, the WAIC does not address issues
arising from the geometry of the parameter space.

Complicating matters is that even when regularity conditions hold at parame-
ters near singularities and boundaries, convergence of the expected AIC may be
slowed, and a generalized form may converge faster to its target. In this sense,
the AICg can be thought of as a finite sample size correction to the standard
AIC. While the AICc \cite{13, 14} also has this interpretation, our generalized form
is more generally applicable.

Alternatives to the AIC include bootstrap variants, introduced by Efron \cite{15,
16}, and further reviewed by Efron and Tibshirani \cite{17}. Ishiguro and Sakamoto \cite{18}
introduced the WIC, while Cavanaugh and Shumway \cite{19}, Shang and Cavanaugh
\cite{20} and Seo and Thorne \cite{21} developed variants for state-space selection, mixed
model selection and partition scheme selection, respectively. To our knowledge,
all existing AIC alternatives and adjustments assume that \( \theta_0 \) is an interior point
of \( \Theta_0 \) and not a singularity or boundary.

The AICg accurately estimates its target, regardless of whether \( \theta_0 \) is a singu-
larity or boundary or not. It is based on Equation 7.53 of Burnham and Anderson
\cite{3}, although issues of singularities and boundaries are not explored in that work.
Indeed, their following Equation 7.54 is not generally correct if the model has
singularities or boundaries.

Derivations of the AIC require a transformation of the space \( \Theta \) that random
observations \( Z_i \) lie in. In the transformation \( \Theta \) is scaled such that random
observations in the transformed space have identity covariance. However, with
covariance that does not converge to the zero matrix in the transformed space,
the MLE is not generally an asymptotically unbiased estimate of the generating
parameter at singularities and boundaries, a necessary condition to progress
from Equation 7.53 to Equation 7.54.

While our AICg is not as simple to use as the AIC, and thus the AIC may
be preferred in standard applications, model singularities and boundaries are
common enough in complex models that our generalized form can provide a useful
improvement in many situations. It highlights the need to consider parameter
space geometry when using the AIC and how this geometry might affect accuracy.

The example models considered in this article are from phylogenomics,
where evolutionary trees relating many species are inferred from genomic data.
Population-genetic effects, such as incomplete lineage sorting modelled by the
multispecies coalescent, result in some inferred gene trees differing from the
overall (generating) species tree. These effects significantly complicate infer-
ence, testing, and model selection of species trees and networks. No technical understanding of these biological processes is required for this article, as these models are all trinomials. Interested readers can consult Mitchell et al. [22] and its appendices for more biological background on our example models, and on hypothesis testing of models with singularities and boundaries.

The article is organized as follows. Section 2 gives definitions, assumptions, and descriptions of example models. The AICg is defined in Section 3 and the proof of the main theorem, that the expected AICg is asymptotically equivalent to its target, is given. In Section 4 the AICg is derived for all example models. Methods for estimating the bias correction, which generally depends on the generating parameter, and for estimating the generating parameter are given in Section 5. To illustrate potential improvements of the AICg, we apply our techniques to example models at and nearby singularities and boundaries and compare performance to the AIC.

2. Definitions, assumptions and models

2.1. Definitions

We define singularities and boundaries of parameter spaces as in Mitchell et al. [22] and Drton [10]. Let $P_{\Theta}$, with $\Theta \subseteq \mathbb{R}^k$, be a parametric family of probability distributions on a measurable space. We assume that the parameter space $\Theta$ is a semialgebraic subset of $\mathbb{R}^k$; that is, it comprises points satisfying a finite collection of multivariate polynomial equalities and inequalities. For a semialgebraic $\Theta_0 \subset \Theta$, we have a subfamily $P_{\Theta_0}$.

A singularity of the parameter space $\Theta_0$ of $P_{\Theta_0}$ is either a) a point in $\Theta_0$ which lies on multiple irreducible algebraic components of $\Theta_0$, or b) a point that lies on only one component, but at which the Jacobian matrix of the defining equations of that component has lower rank than at generic points on the component.

Let $\text{Cl}(\Theta_0)$ denote the Zariski closure of $\Theta_0$; that is, the points satisfying all the equalities defining $\Theta_0$. A subset of $\Theta_0$ is open if it is the intersection of $\text{Cl}(\Theta_0)$ with an open subset of $\mathbb{R}^k$. The interior of $\Theta_0$ is the union of its open subsets, and the boundary of $\Theta_0$ is the complement in $\Theta_0$ of its interior. Note that the boundary and the set of singularities of a model do not need to be disjoint.

We adopt the regularity conditions of Drton [10]: $P_{\Theta}$ is regular at $\theta \in \Theta \subseteq \mathbb{R}^k$ if it satisfies the following conditions: 1) $\theta$ is in the interior of non-empty $\Theta$, 2) The model $P_{\Theta}$ is differentiable in quadratic mean with non-singular Fisher information matrix $I(\theta)$, 3) For all $\theta_1$, $\theta_2$ in a neighborhood of $\theta$ in $\Theta$, $|\log p_{\theta_1}(x) - \log p_{\theta_2}(x)| \leq \tilde{l}(x) \|\theta_1 - \theta_2\|$ for measurable square-integrable function $\tilde{l}$, and 4) The maximum likelihood estimator is a consistent estimator of $\theta$ under $P_{\Theta}$.
2.2. Assumptions

Our models satisfy the following assumptions.

**Assumption A1.** $\mathcal{P}_\theta$ is regular at generating parameter $\theta_0 \in \Theta_0 \subset \Theta \subseteq \mathbb{R}^k$.

**Assumption A2.** $\Theta_0$ is Chernoff regular at $\theta_0$ [23], with maximum likelihood estimator $\hat{\theta}_n$ a consistent estimator of $\theta_0$ under $\mathcal{P}_{\theta_0}$.

**Assumption A3.** $Z_i \in \Theta$, for $i \in \{1, 2, \ldots, n\}$, are i.i.d random observations, with finite expected value $\theta_0$ and non-singular covariance $I(\theta_0)^{-1}$, where $I(\theta_0)$ is the Fisher information matrix for a sample of size 1 and $I(\theta_0)^{\frac{1}{2}}$ a matrix such that $I(\theta_0) = \left( I(\theta_0)^{\frac{1}{2}} \right)^T I(\theta_0)^{\frac{1}{2}}$.

We emphasize that there is no assumption that $\mathcal{P}_{\theta_0}$ is regular at $\theta_0$, only that $\Theta_0$ is Chernoff regular at $\theta_0$. This weaker assumption permits $\theta_0$ to be a singularity and/or boundary of $\Theta_0$. In fact, Chernoff regularity everywhere in $\Theta_0$ is implied by the assumption that $\Theta_0$ is a semialgebraic set [10].

We briefly present and analyze a simple model, illustrating how the expected AIC can fail to converge to its target at a boundary of a parameter space.

**Example 2.1 (AIC for a biased coin toss).** A coin has probability of heads $\theta \in \Theta = (0, 1)$. The submodel $\theta_0 \in \Theta_0 = \left[\frac{1}{2}, 1\right)$, in which heads is at least as likely as tails, has a boundary point at $\theta_0 = \frac{1}{2}$. Assume $n$ is sufficiently large to ignore issues near the boundaries 0 and 1 of $\Theta$.

The target for the expected AIC has asymptotics determined by the tangent cone at $\theta_0$ of $\Theta_0$ and the distribution of $Z_n = \frac{1}{n}Z_n$, asymptotically $\mathcal{N}\left(\theta_0, \frac{1}{n}I(\theta_0)^{-1}\right)$. For any $\theta_0 > \frac{1}{2}$, the tangent cone is a line and the expected AIC converges to its target, with the AIC having bias correction $2k = 2$.

At $\theta_0 = \frac{1}{2}$, the tangent cone is the half-line $\left[\frac{1}{2}, \infty\right)$. Informally, asymptotically with probabilities $\frac{1}{2}$, $\Theta_0$ “behaves” either like a point (when $\hat{\theta}_n = \frac{1}{2}$) or like a line (when $\hat{\theta}_n > \frac{1}{2}$), such that $2k_n = 2 \left(\frac{1}{2} \cdot 0 + \frac{1}{2} \cdot 1\right) = 1$. Thus the expected AIC is not a consistent estimator of its target, which would require AIC bias correction 1 instead of $2k = 2$. In particular, the asymptotics determined by the tangent cone are discontinuous at the boundary point $\theta_0 = \frac{1}{2}$.

Indeed, although the expected AIC converges to its target when $\hat{\theta}_n > \frac{1}{2}$, convergence is slow for parameters near the boundary, when $\theta_0 \approx \frac{1}{2}$. For such $\theta_0$ it is desirable that the bias correction continuously “interpolate” between its value at $\theta_0 = \frac{1}{2}$ and values at regular points far away, but in a way dependent on the sample size $n$ that accurately estimates $2k_n$. This is the goal of developing the generalized AIC.

2.3. Example models

We introduce five models, all trinomial. Four are from phylogenomics, the field of mathematical biology concerned with the inference of evolutionary trees from
genomic-scale data, and a fifth more general model. The four phylogenomics models are based on the multispecies coalescent (MSC) model of incomplete lineage sorting, which can result in different evolutionary relationships on different genes.

For three species, $a$, $b$ and $c$, and three orthologous genes $A$, $B$, $C$, descending from a common ancestral gene, there are three possible rooted gene trees, $A|BC$, $B|AC$ and $C|AB$, describing the gene triplet’s evolutionary history. If an inferred gene tree has topology $B|AC$, for example, then $A$ and $C$ are the two most closely related genes. Assuming the MSC model, the most probable gene tree (rooted triple) topology is the one matching the species tree topology, the overall species history, and the other gene tree triplet probabilities are equal. See Appendix A of Mitchell et al. \cite{22} for a brief, but more thorough, introduction to these trinomial phylogenomic models.

Model $T_1$ posits a specific triplet species tree topology. With $\Theta = \Delta^2$ denoting the open 2-dimensional simplex, its parameter space is the line segment

$$\Theta_0 = \{ p \in \Theta \mid p_1 \geq p_2 = p_3 \},$$

with a boundary at the centroid $\left( \frac{1}{3}, \frac{1}{3}, \frac{1}{3} \right)$ of $\Theta$ corresponding to a “star tree” evolutionary history. Model $T_3$ permits any of the three species tree topologies and has parameter space

$$\Theta_0 = \{ p \in \Theta \mid p_i \geq p_j = p_k, \{i,j,k\} = \{1,2,3\} \},$$

with a singularity at the centroid. The unconstrained model $U$ has $\Delta^2$ as its parameter space, and might be used to model evolution not on a species tree. The polytomy model, modeling a “star tree” where all three species are equally closely related, has the centroid as its parameter space. See Figure 1 for the parameter spaces of the first four models. The fifth more general model is the multiple half-lines model, a specific generalization of $T_1$ and $T_3$. All models satisfy Assumptions A1-A3.

3. A generalized AIC

Common derivations of the AIC, such as that given by Cavanaugh \cite{24}, involve Taylor series in $\theta$ at $\theta_0$ and $\hat{\theta}_n$. Since our interest is in singularities and boundaries, Taylor series fail to exist, and we follow an alternate framework.

For a sample of size $n$, let

$$\Delta_n = \Delta_n (\Theta_0, \theta_0) = \mathbb{E}_0 \left\{ \mathbb{E}_0 \left\{ -2 \log L (\theta ; \mathcal{Z}_n) \right\}_{\theta = \hat{\theta}_n} \right\}.$$  (1)

This is the target for the AIC and AICg. (See Cavanaugh \cite{24} for the connection between the target $\Delta_n$ and the Kullback-Leibler divergence of the approximating model probability distribution at $\hat{\theta}_n$ from the generating model probability distribution at $\theta_0$.)
Fig 1: The models $T_1$ (a) and $T_3$ (b), represented by the solid line segment(s) in $\Delta^2$. The centroid $\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$ is a boundary of model $T_1$ and a singularity of model $T_3$, and also the polytomy model parameter space. All these models are contained in $\Delta^2$, the unconstrained model parameter space.

Cavanaugh [24] derives an unbiased estimator of the target for all $\theta_0 \in \Theta_0$:

$$-2 \log L \left(\hat{\theta}_n | Z_n\right) + E_0 \left\{n \left(\overline{Z}_n - \theta_0\right)^T I \left(\theta_0\right) \left(\hat{\theta}_n - \theta_0\right)\right\}. \tag{2}$$

The expected value of Expression 2 yields the target. Its derivation requires no special assumptions other than well-defined quantities. Our derivation of the AICg approximates the last two terms, the bias correction, in a general way.

**Definition 3.1** (Generalized AIC). For a model meeting the assumptions of Section 2, the generalized AIC for a sample $Z_n = \sum_{i=1}^n Z_i$ of size $n$ is

$$\text{AIC}_g = \text{AIC}_g \left(Z_n, \Theta_0, \theta_0\right) = -2 \log L \left(\bar{\theta}_n | Z_n\right) + 2 E_0 \left\{n \left(\bar{Z}_n - \theta_0\right)^T I \left(\theta_0\right) \left(\bar{\theta}_n - \theta_0\right)\right\}.$$  

**Theorem 3.2.** Under the assumptions of Section 2, $E_0 \{\text{AIC}_g\}$ is asymptotically equivalent to its target $\Delta_n(\Theta_0, \theta_0)$ in the sense that

$$E_0 \{\text{AIC}_g\} - \Delta_n(\Theta_0, \theta_0) \to 0.$$

**Proof.** We focus first on finding an expression for the target $\Delta_n(\Theta_0, \theta_0)$. For an arbitrary $\theta \in \Theta_0$, by the assumptions of Section 2, with $c$ a constant,

$$-2 \log L \left(\theta | Z_n\right) = n \left(\bar{Z}_n - \theta\right)^T I \left(\theta_0\right) \left(\bar{Z}_n - \theta\right) + c + o_p \left(1\right). \tag{3}$$
Let \( A_n \) and \( B_n \) be the random variables on the left and right sides of Equation 3, respectively. With subscripts of zero denoting quantities under the generating process with generating parameter \( \theta_0 \in \Theta_0 \), by Assumption A3, \( \mathbb{E}_0 \{ B_n \} < \infty \), and thus also \( \mathbb{E}_0 \{ A_n \} < \infty \). Thus, \( \mathbb{E}_0 \{ A_n \} = \mathbb{E}_0 \{ B_n \} \) is equivalent to

\[
\mathbb{E}_0 \{ -2 \log L(\theta|Z_n) \} = \mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \theta \right)^T \mathcal{I}(\theta_0) \left( \tilde{Z}_n - \theta \right) \right\} + c + o(1).
\]

Evaluating \( \mathbb{E}_0 \{ A_n \} \) at \( \theta = \theta_0 \) and since \( \hat{\theta}_n \xrightarrow{p} \theta_0 \), then by the continuous mapping theorem,

\[
\mathbb{E}_0 \{ -2 \log L(\theta|Z_n) \}_{|_{\theta=\theta_0}} = \mathbb{E}_0 \{ -2 \log L(\theta|Z_n) \}_{|_{\theta=\hat{\theta}_n}} + o_p(1).
\]

Similarly, for \( \mathbb{E}_0 \{ B_n \} \),

\[
\mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \theta \right)^T \mathcal{I}(\theta_0) \left( \tilde{Z}_n - \theta \right) \right\}_{|_{\theta=\hat{\theta}_n}} + c + o(1).
\]

It follows from \( \mathbb{E}_0 \{ A_n \} = \mathbb{E}_0 \{ B_n \} \) that

\[
\mathbb{E}_0 \{ -2 \log L(\theta|Z_n) \}_{|_{\theta=\hat{\theta}_n}} = \mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \theta \right)^T \mathcal{I}(\theta_0) \left( \tilde{Z}_n - \theta \right) \right\}_{|_{\theta=\hat{\theta}_n}} + c + o_p(1). \tag{4}
\]

Finally, taking the expected value of Equation 4, which is again finite by Assumption A3, we obtain the expression for the target:

\[
\Delta_n(\Theta_0, \theta_0) = \mathbb{E}_0 \left\{ \mathbb{E}_0 \{ -2 \log L(\theta|Z_n) \}_{|_{\theta=\hat{\theta}_n}} \right\}
\]

\[
= \mathbb{E}_0 \left\{ \mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \theta \right)^T \mathcal{I}(\theta_0) \left( \tilde{Z}_n - \theta \right) \right\}_{|_{\theta=\hat{\theta}_n}} \right\} + c + o(1)
\]

\[
= \mathbb{E}_0 \left\{ \mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \theta_0 \right)^T \mathcal{I}(\theta_0) \left( \tilde{Z}_n - \theta_0 \right) \right\}_{|_{\theta=\hat{\theta}_n}} \right\} - 2 \mathbb{E}_0 \left\{ \mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \theta \right)^T \mathcal{I}(\theta_0) (\theta - \theta_0) \right\}_{|_{\theta=\hat{\theta}_n}} \right\}
\]

\[
+ \mathbb{E}_0 \left\{ \mathbb{E}_0 \left\{ n (\theta - \theta_0)^T \mathcal{I}(\theta_0) (\theta - \theta_0) \right\}_{|_{\theta=\hat{\theta}_n}} \right\} + c + o(1).
\]

The quantity simplifies to

\[
\Delta_n(\Theta_0, \theta_0) = \text{dim} (\Theta) + \mathbb{E}_0 \left\{ n \left( \hat{\theta}_n - \theta_0 \right)^T \mathcal{I}(\theta_0) \left( \hat{\theta}_n - \theta_0 \right) \right\} + c + o(1).
\]

Next, focussing on the first term of the AICg, by similar arguments,

\[
\mathbb{E}_0 \{ -2 \log L(\tilde{\theta}_n|Z_n) \} = \mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \hat{\theta}_n \right)^T \mathcal{I}(\theta_0) \left( \tilde{Z}_n - \hat{\theta}_n \right) \right\} + c + o(1)
\]

\[
= \text{dim} (\Theta) - 2 \mathbb{E}_0 \left\{ n \left( \tilde{Z}_n - \theta_0 \right)^T \mathcal{I}(\theta_0) \left( \tilde{Z}_n - \theta_0 \right) \right\}.
\]
\[
+ E_0 \left\{ n \left( \hat{\theta}_n - \theta_0 \right)^T I(\theta_0) \left( \hat{\theta}_n - \theta_0 \right) \right\} + c + o(1),
\]
where \( c \) is the same constant as in Equation 3.

The result then follows.

Under the assumptions of Section 2, the second term of the AICg is asymptotically equivalent to the bias correction (last two terms) of Expression 2.

An equivalent expression that may be easier to compute for some models is

\[
\text{AICg} = -2 \log L \left( \hat{\theta}_n | Z_n \right) + \dim(\Theta) + E_0 \left\{ n \left( \hat{\theta}_n - \theta_0 \right)^T I(\theta_0) \left( \hat{\theta}_n - \theta_0 \right) \right\} + E_0 \left\{ n \left( \bar{Z}_n - \hat{\theta}_n \right)^T I(\theta_0) \left( \bar{Z}_n - \hat{\theta}_n \right) \right\}.
\]

Remark 1. To derive the AICg for specific models more easily, we apply a linear transformation \( \Theta \mapsto \sqrt{n} I(\theta_0)^{1/2} \Theta \) to the bias correction. Under this transformation, \( \Theta \mapsto M, \theta_0 \mapsto M_0, \hat{\theta}_n \mapsto \hat{\mu}_n, \bar{Z}_n \mapsto \bar{z}_n \) and \( \bar{z}_n \) converges in distribution to \( z \sim N(\mu_0, I) \), where \( I \) is the identity matrix. After this transformation to the bias correction,

\[
\text{AICg} = -2 \log L \left( \hat{\theta}_n | Z_n \right) + 2E_0 \left\{ (\bar{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) \right\}.
\]

The value \( ||\mu_0|| \) has a simple interpretation: It represents the Mahalanobis distance between the generating parameter \( \theta_0 \) and a singularity or boundary, which is defined to be at the origin. For models with one parameter, \( ||\mu_0|| \) is the number of standard deviations of \( \bar{Z}_n \) between \( \theta_0 \) and the singularity or boundary.

Moreover, asymptotically this bias correction is non-negative, which we prove.

Proposition 3.3. For a model satisfying the assumptions of Section 2, asymptotically the bias correction of Equation 5 is non-negative. Specifically,

\[
2E_0 \left\{ (\bar{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) \right\} \geq 0.
\]

Proof. We prove that

\[
(\bar{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) = (\bar{z}_n - \mu_0) \cdot (\hat{\mu}_n - \mu_0) \geq 0.
\]

If the dot product is negative, then considering the lengths of the triangle with vertices \( \bar{z}_n, \mu_0 \) and \( \hat{\mu}_n \), we find that \( ||\bar{z}_n - \mu_0|| < ||\bar{z}_n - \hat{\mu}_n|| \), a contradiction since \( \hat{\mu}_n \) is the maximum likelihood estimate.

4. Applications of the AICg to example models

In this section we derive explicit formulas for the AICg for example models \( T1, T3 \) and the multiple half-lines model. Since the example models consist of half-open line segments in \( \Delta^2 \) with interesting geometry at the centroid \( \theta_0 = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \), we replace these line segments with half-lines extending from \( \theta_0 \) and \( \Delta^2 \) with \( \mathbb{R}^2 \). Furthermore, we assume random observations are multivariate normally distributed, as they are asymptotically.
4.1. Model \( T_1 \)

The linear transformation of Remark 1 and extension of parameter spaces projects \( \Theta = \Delta^2 \) onto \( \mathbb{R}^2 \), with \( M_0 = \mathbb{R}^+ \), \( \mu_0 = (0, \mu_{0,y}) \) and \( \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) \mapsto (0,0) \).

Defining \( \phi_0 \in (0,1] \) via \( p_1 = 1 - \frac{2}{3} \phi_0 \), then from Mitchell et al. \[22\], \( \mu_{0,y} = \sqrt{2n} \frac{1 - \phi_0}{\phi_0 (3 - 2\phi_0)} \).

**Proposition 4.1.** For model \( T_1 \),

\[
\text{AIC}_g = -2 \log L \left( \hat{\theta}_n | Z_n \right) + 1 + \text{erf} \left( \frac{\mu_{0,y}}{\sqrt{2}} \right).
\]

**Proof.** Let \( w = (x,y)^T \) be an arbitrary realization of \( \bar{z}_n \) in \( M \), and \( m_0 = (0,m_{0,y})^T \) the point of \( M_0 \) closest to \( w \) in Euclidean distance.

When \( y < 0 \), \( m_0 = (0,0)^T \) and thus \( (w - \mu_0)^T (m_0 - \mu_0) = -\mu_{0,y} (y - \mu_{0,y}) \).

When \( y \geq 0 \), \( m_0 = (0,y)^T \) and \( (w - \mu_0)^T (m_0 - \mu_0) = (y - \mu_{0,y})^2 \).

Then the \( \text{AIC}_g \) bias correction is

\[
2 \mathbb{E}_0 \left\{ (\bar{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) \right\} = 2 \int_{-\infty}^{0} -\mu_{0,y} (y - \mu_{0,y}) \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{1}{2} (y - \mu_{0,y})^2 \right) dy + 2 \int_{0}^{\infty} (y - \mu_{0,y})^2 \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{1}{2} (y - \mu_{0,y})^2 \right) dy = 1 + \text{erf} \left( \frac{\mu_{0,y}}{\sqrt{2}} \right).
\]

\[\square\]

In Figure 2 we compare the performance of the \( \text{AIC}_g \) bias correction with known \( \mu_{0,y} \), the AIC bias correction, and their target. Since the \( \text{AIC}_g \) depends on \( \mu_{0,y} = \mu_{0,y}(n) \), we make these comparisons for sample sizes \( n \in \{30, 100, 1000\} \). For estimating the target, which is challenging to determine in closed form, we averaged \( 10^7 \) simulations for each \( \mu_{0,y} \in \{0, 0.02, 0.04, \ldots, 5\} \) and fitted a cubic smoothing spline. We see that the \( \text{AIC}_g \) bias correction quickly converges to its target, accurately interpolating from 1 (corresponding to an effective number of parameters \( k_e = \frac{1}{2} < 1 = k \)) at the boundary point to 2 (for effective number of parameters \( k_e = 1 = k \)) at points infinitely far from the boundary. The interpolating feature of the \( \text{AIC}_g \) addresses in a sample-size dependent way the practical concern of computing effective numbers of parameters at generating parameters near the boundary. By way of contrast, note that (except for when \( n \) is small) the AIC always overestimates the bias correction \( (k > k_e) \), with the magnitude of the error particularly large at points near the boundary \( \mu_{0,y} = 0 \), since it assigns a constant bias correction of 2. The AIC also converges slowly to the target, requiring a Mahalanobis distance of \( \mu_{0,y} \approx 2 \) or more from the boundary for accurate performance.
4.2. Model $T_3$

Again using the transformation of Remark 1 and extension of parameter spaces, model $T_3$ maps to three rays in $\mathbb{R}^2$ emanating from (0, 0). They are the non-negative $y$-axis and rays in quadrants 3 and 4 forming an angle $\alpha_0$ with the negative and positive $x$-axis respectively. If $\theta_0 = (p_1, p_2, p_3)$, then with $p_i$ maximal for some $i \in \{1, 2, 3\}$, $\phi_0 \in (0, 1]$ satisfies $p_i = 1 - \frac{2}{3} \phi_0$. With no loss of generality, we assume $\mu_0 = (0, \mu_{0,y})$ lies on the non-negative $y$-axis. After transformation, the bias correction depends on $\mu_{0,y} = \mu_{0,y}(n)$ and $\alpha_0 = \arctan\left(\frac{1}{\sqrt{3(3 - 2\phi_0)}}\right)$, with $\beta_0 = \frac{1}{2} \left(\frac{\pi}{2} - \alpha_0\right)$.

**Proposition 4.2.** For model $T_3$,

\[
AIC_g = -2 \log L \left( \hat{\theta}_n | Z_n \right) + \frac{\sqrt{3}}{\pi} \int_0^\infty (y - \mu_{0,y})^2 \exp \left( -\frac{1}{2} (y - \mu_{0,y})^2 \right) \text{erf} \left( \frac{y \cot \beta_0}{\sqrt{2}} \right) dy + 2 \pi \int_{-\pi}^{\beta_0} \int_0^\infty g \exp \left( -\frac{1}{2} (r^2 - 2\mu_{0,y} r \sin \phi + \mu_{0,y}^2) \right) dr d\phi,
\]

where

\[
g = g(r, \phi, \mu_{0,y}, \alpha_0) = r \left( r^2 \cos^2 (\phi + \alpha_0) - \mu_{0,y} r (\sin \phi - \sin \alpha_0 \cos (\phi + \alpha_0)) + \mu_{0,y}^2 \right).
\]

See Appendix A for the proof.

Although the inner integral of the second term of the bias correction can be evaluated in closed form, the bias correction as given here is quickly and easily evaluated by numerical integration.
Fig 3: Performance of AICg bias correction (blue) and AIC bias correction (red) compared to their target estimated by simulation (black) for model $T_3$.

In Figure 3 we compare the performances of the AICg bias correction, the AIC bias correction, and the approximated target for $\mu_{0,y}$ known. The target is estimated with the same method as for model $T_1$. The AICg bias correction again quickly converges to its target, accurately interpolating from $2 + \frac{3\sqrt{3}}{2\pi}$ (for effective number of parameters $k_e = 1 + \frac{3\sqrt{3}}{2\pi} > k$) at the singularity $(0,0)$ to $2$ (for effective parameters $k_e = 1 = k$) infinitely far from the singularity. Convergence of the AIC is particularly slow at generating parameters near the parameter space singularity. Interestingly, while the AIC underestimated its target for model $T_1$, for this model the AIC overestimates, illustrating that effective number of parameters can be smaller or larger than $\text{dim}(\Theta_0)$.

4.3. Multiple half-lines model

It is instructive to consider a generalization of the $T_1$ and $T_3$ models, composed of many half-lines in a plane meeting at a singularity. This sheds light on how the angles between these lines influence the bias correction, and thus the notion of effective number of parameters at their meeting point. We assume $M_0 \subset \mathbb{R}^2$ is the union of $l \geq 1$ half-lines emanating from $(0,0)$.

**Proposition 4.3.** Suppose $M_0$ for the multiple half-lines model has $l \in \mathbb{Z}^+$ half-lines, rays at angles $0 < \alpha_1 < \ldots < \alpha_l = 2\pi$ counter-clockwise from the non-negative $x$-axis, with the largest sector that between the non-negative $x$-axis and the ray $\alpha_1$. For each $i \in \{1, 2, \ldots, l\}$, let $\varphi_i = \alpha_i - \alpha_{i-1}$, with $\alpha_0 = 0$. Then at $\mu_0 = (0,0)$,

$$\text{AIC}_g = \begin{cases} 
-2\log L(\hat{\theta}_n|Z_n) + 2 + \frac{1}{\pi} \sum_{i=1}^{l} \sin (\varphi_i), & \text{if } \varphi_1 \in (0, \pi], \\
-2\log L(\hat{\theta}_n|Z_n) + 3 + \frac{1}{\pi} \left( \sum_{i=2}^{l} \sin (\varphi_i) - \varphi_1 \right), & \text{if } \varphi_1 \in (\pi, 2\pi]. 
\end{cases}$$

For a proof, see Appendix B.
The following corollaries, for the special case that all angles $\varphi_i$ are equal, follow easily.

**Corollary 4.4.** Let $\varphi_i = \frac{2\pi}{l}$ for all $i \in \{1, 2, \ldots, l\}$. Then

\[
AICg = \begin{cases} 
-2 \log L \left( \theta_n | Z_n \right) + 1, & \text{if } l = 1, \\
-2 \log L \left( \theta_n | Z_n \right) + 2 + \frac{l}{\pi} \sin \left( \frac{2\pi}{l} \right), & \text{if } l \in \{2, 3, \ldots\}.
\end{cases}
\]

**Corollary 4.5.** Let $\varphi_i = \frac{2\pi}{l}$ for all $i \in \{1, 2, \ldots, l\}$. Then as $l \to \infty$,

\[
AICg \to -2 \log L \left( \tilde{\theta}_n | Z_n \right) + 4.
\]

**Remark 2.** Note that models $T1$ ($l = 1$) and $T3$ ($l = 3$) are special cases of the multiple half-lines model, when the generating parameter is the boundary/singularity of the parameter space. Moreover, as $l \to \infty$, as in the preceding corollary, we obtain the unconstrained model $U$. An easy extension to the case that $l = 0$ yields the polytomy model, with a single point parameter space. Since both the polytomy model and $U$ are regular (no singularities or boundaries) and linear at all points, the AIC and the AICg coincide for these models.

In the phylogenomics applications motivating this work, empiricists might use model selection to choose between a particular rooted triple, say $abc$ (in which species $b$ and $c$ are most closely related), and a star tree showing no pair of the three most closely related. This requires selecting between model $T1$ and the polytomy model. Similarly, AICg model selection might be used to choose between relating three species with rooted tree ($T3$), or rejecting tree-like evolution if the unconstrained model $U$ is selected. In Figure 4 we show AICg model selection results for a sample of size $n = 200$, when $\hat{\mu}_0$ is used to evaluate the bias correction.

5. Using the AICg in practice

As the AICg bias correction may be a function of the unknown generating parameter, practical means for estimating the parameter or directly estimating the bias correction are needed. We restrict ourselves to the transformed basis introduced in Remark 1 as the generating parameter and bias correction are typically easiest to estimate in this basis.

The simplest solution, using the AICg and estimating $\mu_0$ with $\hat{\mu}_n$, often results in a much more accurate estimate of the target than the AIC does, yet, like the AIC, the AICg with $\hat{\mu}_n$ is not generally a consistent estimator of the target at singularities and boundaries. In this section we outline several methods that might be used to estimate bias corrections in practice. In addition to the AIC bias correction and AICg bias correction computed with the MLE, these include least favorable bias corrections, uniformly outperforming bias corrections and minimax bias corrections. We illustrate how these bias corrections might perform,
Fig 4: Model selection outcomes based on the AICg using $\hat{\mu}_n$ and $n = 200$. (a) For observations in the blue region, Model $T_1$ is selected; for observations in green, the polytomy model is selected. (b) Model $T_3$ is selected for observations in the blue region; the unconstrained model $U$ is selected in the green region.

by comparing and contrasting them to the AIC bias correction and AICg bias correction with known parameter for example models $T_1$ and $T_3$. We conclude with a brief discussion of consistent bias corrections and how our ideas might extend to more complicated models.

5.1. Some practical bias corrections

5.1.1. Lower and upper least favorable bias corrections

Least favorable bias corrections are inspired by the least favorable method of hypothesis testing, dating back to at least Self and Liang [25]. The lower/upper least favorable bias corrections $c_{llf}/c_{ulf}$ correspond to the infimum/supremum of the bias corrections over $M_0$.

5.1.2. Uniformly outperforming bias corrections

Uniformly outperforming bias corrections $c_{uo}$ are those that outperform the AIC bias correction; that is, if $c_{uo}$ has bias, it has the same sign as the bias of the AIC bias correction everywhere in $M_0$, but with smaller magnitude. One such construction is to consider neighborhoods of fixed radii around each singularity and boundary in $M_0$, with the radii chosen to satisfy the uniformly outperforming criterion. More specifically, if $\hat{\mu}_n$ or $\bar{z}_n$ lies inside a neighborhood, then the bias correction is taken to be that at the singularity/boundary within the neighborhood. Otherwise, the bias correction is that of the AIC. If $\hat{\mu}_n$ or $\bar{z}_n$ lies inside multiple neighborhoods, then the neighborhood of the singularity/boundary closest in Euclidean distance is used, with ties settled at random.
5.1.3. Minimax bias corrections

Minimax bias corrections $c_m$ are similar to uniformly outperforming bias corrections, except that the radii of singularity/boundary neighborhoods are chosen to minimize the supremum of a risk function over $\mathcal{M}_0$. In the comparisons we make below, we choose the risk function to be the $L^2$ norm between the “true” bias correction from known $\mu_0$ and the expected estimated bias correction from the method described with neighborhoods enclosing singularities and boundaries.

In practice, to determine whether a bias correction is least favorable, uniformly outperforming or minimax, we typically assume $n$ is sufficiently large for the AICg bias correction with known $\mu_0$ to accurately approximate the “true” bias correction.

5.2. Comparison of bias corrections for models $T_1$ and $T_3$

The least favorable bias corrections for model $T_1$ are 1, corresponding to $\mu_{0,y}, y = 0$, and 2, as $\mu_{0,y} \to \infty$. A simple uniformly outperforming bias correction is $c_u = 1$ if $\hat{\mu}_{n,y} = 0$, and $c_u = 2$ otherwise, since $1 + \text{erf} \left( \frac{\mu_{0,y}}{\sqrt{2}} \right) < \mathbb{E}_0 \{ c_u \} < 2$.

Our minimax bias correction is $c_m = 1$ if $\hat{\mu}_{n,y} \leq 0.95$, and $c_m = 2$ otherwise.

For model $T_3$, the least favorable bias corrections are 2 ($\mu_{0,y} \to \infty$) and $2 + \frac{3\sqrt{3}}{2\pi} (\mu_{0,y} = 0)$. Finding a strictly uniformly outperforming bias correction for model $T_3$ is challenging, however. Instead, we use a bias correction for $T_3$ that almost uniformly outperforms the AIC bias correction, which we still refer to as the uniformly outperforming bias correction. The uniformly outperforming bias correction and the AIC bias correction are permitted to have opposite sign biases if the bias of the uniformly outperforming bias correction has small magnitude.

The AICg bias correction depends on $n$ in multiple ways, not only through $\mu_{0,y} = \mu_{0,y}(n)$. Thus, we set $n = 10^6$ so that the AICg bias correction closely approximates its target and base all other bias corrections off $n = 10^6$. With this procedure, $c_u = 2 + \frac{3\sqrt{3}}{2\pi} \text{ if } \| \bar{z}_n \| \leq r$ and $c_u = 2$ otherwise. Setting the radius $r = 1.77$ ensures that if the uniformly outperforming bias correction and AIC bias correction have different sign biases, the magnitude of the bias of the uniformly outperforming bias correction does not exceed $1.02 \times 10^{-14}$. For the minimax bias correction $c_m$, we use the same procedure with $r = 2.21$.

In Figure 5, we compare the performances of these bias corrections for models $T_1$ and $T_3$ under the assumption that the AICg bias correction with known $\mu_{0,y}$ closely approximates its target. The lower and upper least favorable corrections sandwich all other bias corrections, and the AIC bias correction is the upper least favorable for $T_1$ and the lower least favorable for $T_3$. These are the worst performing bias corrections, in the sense that they deviate most markedly from the blue curve, the bias correction of the AICg with known $\mu_0$, which well approximates the target. Of the data dependent bias corrections, the bias correction of the AICg using $\hat{\mu}_n$, whose expectation was estimated by averaging $10^7$ simulations for each $\mu_{0,y} \in \{0, 0.02, 0.04, \ldots, 5\}$, is perhaps the easiest to use for these models and performs well.
5.3. Consistent bias corrections

In circumstances that the sample size $n$ can be chosen before an experiment is performed, a consistent bias correction method may be preferable, with $n$ chosen sufficiently large to ensure a desired accuracy. Such an estimator could be obtained using similar procedures to the first method of Andrews [26]. This method is similar to the methods for obtaining uniformly outperforming and minimax bias corrections, except radii of neighborhoods increase with $n$ in such a way that $\hat{\mu}_n$ or $\bar{z}_n$ converge almost surely to be inside/outside a neighborhood if $\mu_0$ is/is not the singularity or boundary inside the ball.

The radii are chosen to increase with $n$ more slowly than $\mu_0$ for generic parameters; that is, more slowly than $O(\sqrt{n})$. Suppose $\mu^\dagger$ is the closest singularity or boundary to $\hat{\mu}_n$ or $\bar{z}_n$. Then $\mu_0$ is estimated by the singularity or boundary if $\|\hat{\mu}_n - \mu^\dagger\| \leq \sqrt{n}\eta_n$ or $\|\bar{z}_n - \mu^\dagger\| \leq \sqrt{n}\eta_n$, where $\sqrt{\log \log n} < O(\eta_n) < 1$.

The second method of Andrews [26] can also be adapted to consistently estimate the target using a parametric bootstrap. For this, first obtain a consistent estimate $\tilde{\mu}_n$ of $\mu_0$, as in the first method above. Then generate parametric bootstraps $\tilde{z}_n^* \sim N(\tilde{\mu}_n, I)$. For each bootstrap, estimate the generating parameter $\tilde{\mu}_n^*$ as described in the first method above. Then take the bias correction to be $(\tilde{z}_n^* - \tilde{\mu}_n)^T (\tilde{\mu}_n^* - \tilde{\mu}_n)$. Finally, average this quantity over all bootstrap replicates to obtain the estimate of the AICg bias correction.
5.4. **Estimating the bias correction in complicated models**

The AICg bias correction can be difficult to determine for complicated models. In these circumstances the AIC might be preferable. This requires a rigorous justification, and one should establish that $\theta_0$ is likely to be far from any singularity or boundary, or that the expected AIC is still an accurate estimator of its target, despite the presence of singularities or boundaries.

For estimating the proximity of $\theta_0$ to any singularity or boundary, one might use the Mahalanobis distances from $\hat{\theta}_n$ or $\bar{Z}_n$ to singularities/boundaries (equivalently, the Euclidean distance from $\hat{\mu}_n$ or $\bar{z}_n$), which can be estimated by parametric or non-parametric bootstrapping. As an alternative, one might conclude that $\theta_0$ is likely far from all singularities or boundaries if the proportion of parametric or non-parametric bootstrap maximum likelihood estimates on the same irreducible component of $\Theta_0$ is high.

When one cannot justify using the AIC and the AICg is difficult to compute, crude bounds on the AICg bias correction may be more practical. These bounds may be sufficient for model selection, even if they are not infima/suprema, particularly when the maximum likelihood term of the AIC/AICg differs substantially between models, making the bias correction of little consequence. Lower/upper bounds could be obtained by replacing $\Theta_0$ with affine subspaces/superspaces, and estimating the bias correction by twice the dimension of the space. In a similar vein, $\Theta_0$ could be replaced by spaces with desirable geometric properties, such as half-spaces or orthants, and the bias correction estimated. From Proposition 3.3, we conclude that asymptotically one such lower bound for all models is 0. In short, careful consideration of models and their geometries should be undertaken before determining whether to use the AIC.

6. **Discussion**

Despite being common in practical applications, the effect that singularities and boundaries have on the accuracy of the AIC has not received sufficient attention in the literature to date. Best practice should include attempts to determine whether regularity conditions are satisfied and, if not, the effect of their violation on the accuracy of the AIC. We emphasize the importance of establishing that the AIC consistently estimates its target. If the AIC does not consistently estimate its target or accuracy cannot be quantified, the AICg may be a more appropriate alternative. Estimating the bias correction via bootstrap procedures or crude bounds are both fairly accessible. Crude bounds could be interpreted as being analogous to conservative hypothesis testing procedures; a crude lower/upper bound could be chosen if one wants to preference that model more/less relative to other models.

Indeed as shown here, consideration of the parameter space geometry and its consequences on model selection performance for generating parameters at or near singularities and boundaries can facilitate more accurate model selection practices. In contrast to the AIC, the expected AICg is a consistent estimator of
its target at singularities and boundaries and can converge more quickly than the AIC elsewhere.

Other model selection procedures, such as the Bayesian information criterion (BIC) [27], as well as cross-validation, may perform poorly in the presence of singularities and boundaries. Generalized versions may also be more appropriate.

Methods described here may be more appropriate for models with high curvature at generating parameters that are not singularities or boundaries. For such geometry the AIC may converge slowly. Large $n$ may be required for $\Theta_0$ to be approximately locally linear and for the AIC to be accurate.

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Appendix A: Derivation of AICg for Model T3

Proof of Proposition 4.2. Without loss of generality assume that $\mu_0 = (0, \mu_{0,y})$ lies on the vertical half-line of model T3. Since $\mathcal{M}_0$ is symmetric about the $y$-axis, to determine the bias correction we integrate only over the right half-plane $x > 0$, then multiply the result by 2. To accomplish this integration, $2E_0 \left\{ (\bar{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) \right\}$, we divide the right half-plane into two regions, $y > x \tan \beta_0$ and $y < x \tan \beta_0$, since $\bar{z}_n$ is closer to the vertical model line segment in the first region, and to the model line segment in Quadrant IV in the second region. (These are the same angles and model half-lines of Figure 12 of Mitchell et al. [22].)

Using the notation as in the proof of Proposition 4.1, when $w = (x, y)^T$ is in the first region, the closest model point is $m_0 = (0, y)^T$ and $(w - \mu_0)^T (m_0 - \mu_0) = (y - \mu_{0,y})^2$. In this region,

$$2E_0 \left\{ (\bar{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) \right\} = 4 \int_0^\infty \int_0^{y \cot \beta_0} (y - \mu_{0,y})^2 \frac{1}{2\pi} \exp \left( -\frac{1}{2} \left( x^2 + (y - \mu_{0,y})^2 \right) \right) dx dy$$

$$= \sqrt{\frac{2}{\pi}} \int_0^\infty (y - \mu_{0,y})^2 \exp \left( -\frac{1}{2} (y - \mu_{0,y})^2 \right) \operatorname{erf} \left( \frac{y \cot \beta_0}{\sqrt{2}} \right) dy.$$

When $w$ is in the second region, where $y < x \tan \beta_0$, since $\alpha_0$ is acute, the closest model point is $m_0 = (x_0, -x_0 \tan \alpha_0)$, with $x_0$ to be determined. Using polar coordinates for $\bar{z}_n$, let $r = \sqrt{x^2 + y^2}$ and $\varphi \in (\pi, 2\pi) = \arctan \left( \frac{y}{x} \right)$. With this notation, the angle between $m_0$ and $\bar{z}_n$ (viewed as vectors) is $\varphi + \alpha_0$. Thus, $x_0 = (r \cos(\varphi + \alpha_0)) \cos \alpha_0$ and $y_0 = (r \cos(\varphi + \alpha_0)) \sin \alpha_0$. Thus,

$$(w - \mu_0)^T (m_0 - \mu_0)$$
\[
\begin{align*}
&= \left[ r \cos \varphi \sin \varphi - \mu_{0,y} \right] \left[ \begin{array}{c}
 r \cos (\varphi + \alpha_0) \cos \alpha_0 \\
 -r \cos (\varphi + \alpha_0) \sin \alpha_0 - \mu_{0,y}
\end{array} \right] \\
= & r^2 \cos^2 (\varphi + \alpha_0) - \mu_{0,y} r (\sin \varphi - \sin \alpha_0 \cos (\varphi + \alpha_0)) + \mu_{0,y}^2.
\end{align*}
\]

It follows that, in this region,
\[
\begin{align*}
&\frac{\partial}{\partial \alpha_0} \mathbb{E}_0 \{ (\tilde{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) \} \\
&= \frac{2}{\pi} \int_{-\pi/2}^{\alpha_0} \int_0^\infty r \left( r^2 \cos^2 (\varphi + \alpha_0) - \mu_{0,y} r (\sin \varphi - \sin \alpha_0 \cos (\varphi + \alpha_0)) + \mu_{0,y}^2 \right) \\
&\quad \exp \left( -\frac{1}{2} r^2 - 2 \mu_{0,y} r \sin \varphi + \mu_{0,y}^2 \right) dr d\varphi.
\end{align*}
\]

The result then follows.

\[\square\]

**Appendix B: Derivation of the AICg for the multiple half-lines model**

**Proof of Proposition 4.3.** We use the same notation as in the proof of Proposition 4.1. We compute \(2 \mathbb{E}_0 \{ (\tilde{z}_n - \mu_0)^T (\hat{\mu}_n - \mu_0) \} = 2 \mathbb{E}_0 \{ \tilde{z}_n^T \hat{\mu}_n \} \) when \( \mu_0 = 0 \), by integrating over sectors of the plane of measure \( \varphi_i \).

The value of the AICg depends on the measure of \( \varphi_1 \), and we suppose first that \( \varphi_1 \in (0, \pi] \) and that \( w = (x, y) = (r \cos \theta, r \sin \theta) \) is a realization of \( \tilde{z}_n \) in the first sector \( R_1 \), where \( \theta \in [0, \varphi_1] \). The closest model point \( m_0 \) is on the non-negative \( x \)-axis if \( \theta \in [0, \varphi_1/2] \), and on \( \alpha_1 \) if \( \theta \in [\varphi_1/2, \varphi_1] \). When \( \theta \in [0, \varphi_1/2] \), \( m_0 = (x, 0) = (r \cos \theta, 0) \). When \( \theta \in [\varphi_1/2, \varphi_1] \), \( m_0 = (r \cos (\varphi_1 - \theta) \cos \varphi_1, r \cos (\varphi_1 - \theta) \sin \varphi_1) \).

Thus, over this sector, with area element \( dA \), we find
\[
2 \int_{R_1} \tilde{z}_n^T \hat{\mu}_n \frac{1}{2\pi} \exp \left( -\frac{1}{2} (x^2 + y^2) \right) dA
= \frac{1}{\pi} \left[ \int_0^{\varphi_1/2} \cos^2 \theta d\theta + \int_{\varphi_1/2}^{\varphi_1} \cos^2 (\varphi_1 - \theta) d\theta \right] \int_0^\infty r^3 \exp \left( -\frac{1}{2} r^2 \right) dr
= \frac{1}{\pi} \left[ 2 \left( \frac{\varphi_1}{4} + \frac{\sin \varphi_1}{4} \right) \right] \cdot 2
= \frac{1}{\pi} (\varphi_1 + \sin \varphi_1).
\]

Since \( \varphi_i \leq \varphi_1 \leq \pi \) for all \( i \in \{2, 3, \ldots, l\} \), and the Gaussian density is symmetric about the origin, we find that
\[
2 \mathbb{E}_0 \{ \tilde{z}_n^T \hat{\mu}_n \} = \sum_{i=1}^{l} \frac{1}{\pi} (\varphi_i + \sin \varphi_i) = 2 + \frac{1}{\pi} \sum_{i=1}^{l} \sin \varphi_i.
\]
For the second case, $\varphi_i \in (\pi, 2\pi]$. Then $\varphi_i \in (0, \pi)$ for all $i \in \{2, 3, \ldots, l\}$. If $w = (r \cos \theta, r \sin \theta)$, then the model point $m_0 = (0, 0)$ is closest to $w$ if $\varphi_1 \in \left[\frac{\pi}{2}, \varphi_1 - \frac{\pi}{2}\right]$. When $\theta \in (0, \frac{\pi}{2}]$, then as above

$$2 \int_0^{\frac{\pi}{2}} \int_0^{\infty} \bar{z}_n^T \hat{\mu}_n \frac{1}{2\pi} \exp \left(-\frac{1}{2} r^2\right) rdrd\theta = \frac{1}{\pi} \left(\frac{\pi}{4} + \sin (\pi)\right) \cdot 2 = \frac{1}{2}.$$ 

Again using that the Gaussian is symmetric, integrating over $\theta \in \left[\varphi_1 - \frac{\pi}{2}, \varphi_1\right]$ also yields the value $\frac{1}{2}$. Thus, when $\varphi_1 \in (\pi, 2\pi]$,

$$2 \mathbb{E}_0 \left(\bar{z}_n^T \hat{\mu}_n\right) = \sum_{i=2}^{l} \frac{1}{\pi} \left(\varphi_i + \sin \varphi_i\right) + 2 \cdot \frac{1}{2} = 3 + \frac{1}{\pi} \left(\sum_{i=2}^{l} \sin \varphi_i - \varphi_1\right).$$

\[\square\]

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