Akaike Information Criterion

Shuhua Hu
Center for Research in Scientific Computation
North Carolina State University
Raleigh, NC

Background

- **Model**

  statistical model: $X = h(t;q) + \epsilon$

  - h: mathematical model such as ODE model, PDE model, algebraic model, etc.
  - ϵ: random variable with some probability distribution such as normal distribution.
  - X is a random variable.

  Under the assumption of ϵ being i.i.d $N(0, \sigma^2)$, we have

  probability distribution model: $g(x|\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-h(t;q))^2}{2\sigma^2}\right]$, where $\theta = (q, \sigma)$.

  - g: probability density function of x depending on parameter θ.
  - θ includes mathematical model parameter q and statistical model parameter σ.

- **Risk**

  - **“Modeling” error (in terms of uncertainty assumption)**

    Specified inappropriate parametric probability distribution for the data at hand.

▼ Estimation error

$$\|\vartheta - \hat{\theta}\|^2 = \underbrace{\|\vartheta - \theta\|^2}_{\text{bias}} + \underbrace{\|\theta - \hat{\theta}\|^2}_{\text{variance}}$$

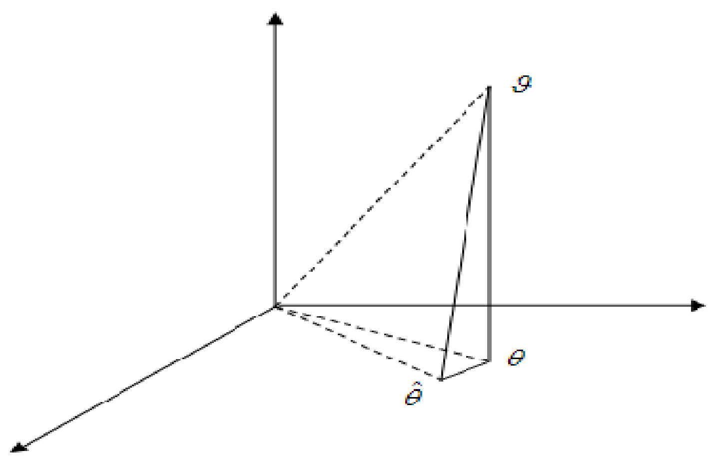
ϑ: parameter vector for the full reality model.

θ: is the projection of ϑ onto the parameter space of the approximating model Θ^k.

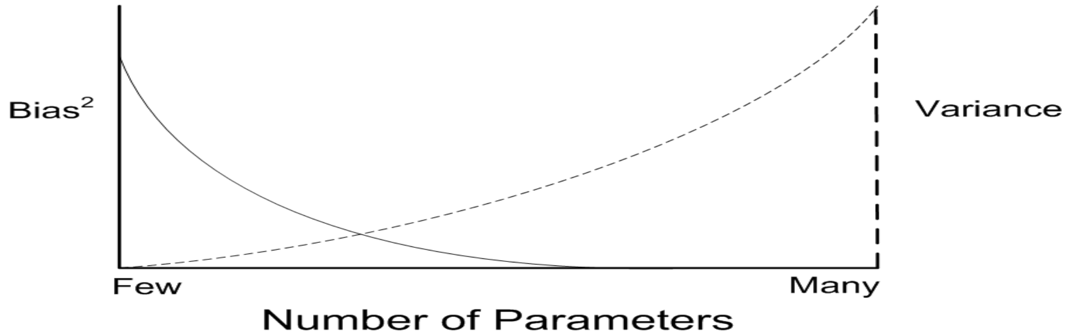
$\hat{\theta}$: the maximum likelihood estimate of θ in Θ^k.

▶ Variance

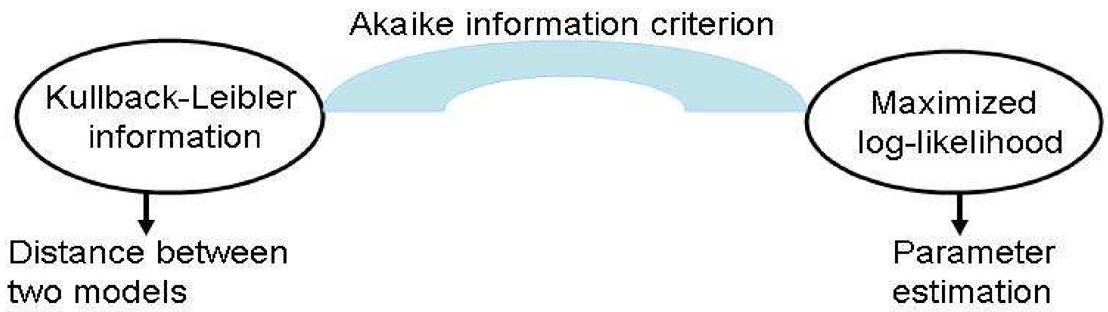
For sufficiently large sample size n, we have $n\|\theta - \hat{\theta}\|^2 \overset{assym.}{\sim} \chi^2_k$, where $E(\chi^2_k) = k$.



- **Principle of Parsimony** (*with same data set*)



- **Akaike Information Criterion**



Kullback-Leibler Information

Information lost when approximating model is used to approximate the full reality.

- **Continuous Case**

$$
\begin{aligned}
I(f, g(\cdot|\theta)) &= \int_\Omega f(x) \log\left(\frac{f(x)}{g(x|\theta)}\right) dx \\
&= \int_\Omega f(x)\log(f(x))dx - \underbrace{\int_\Omega f(x)\log(g(x|\theta))dx}_{\text{relative K-L information}}
\end{aligned}
$$

  - ▼ f: full reality or truth in terms of a probability distribution.
  - ▼ g: approximating model in terms of a probability distribution.
  - ▼ θ: parameter vector in the approximating model g.

- **Remark**

  - ▼ $I(f, g) \geq 0$, with $I(f, g) = 0$ if and only if $f = g$ almost everywhere.
  - ▼ $I(f, g) \neq I(g, f)$, which implies **K-L information is not the real "distance"**.

Akaike Information Criterion (1973)

- **Motivation**
  - ▼ The truth f is unknown.
  - ▼ The parameter θ in g must be estimated from the empirical data y.
    - ▶ Data y is generated from $f(x)$, i.e. realization for random variable X.
    - ▶ $\hat{\theta}(y)$: estimator of θ. It is a random variable.
    - ▶ $I(f, g(\cdot|\hat{\theta}(y)))$ is a random variable.
  - ▼ **Remark**
    - ▶ We need to use expected K-L information $E_y[I(f, g(\cdot|\hat{\theta}(y)))]$ to measure the "distance" between g and f.

- **Selection Target**

$$\underset{g\in G}{\text{Minimizing}}\ E_y[I(f, g(\cdot|\hat{\theta}(y)))]$$

▼ $E_y[I(f, g(\cdot|\hat{\theta}(y)))] = \int_\Omega f(x)\log(f(x))dx - \underbrace{\int_\Omega f(y)\left[\int_\Omega f(x)\log(g(x|\hat{\theta}(y)))dx\right]dy}_{E_yE_x[\log(g(x|\hat{\theta}(y)))]}.$

▼ G: collection of "admissible" models (in terms of probability density functions).

▼ $\hat{\theta}$ is MLE estimate based on model g and data y.

▼ y is the random sample from the density function $f(x)$.

- **Model Selection Criterion**

$$\underset{g\in G}{\text{Maximizing}}\ E_yE_x[\log(g(x|\hat{\theta}(y)))]$$

- **Key Result**

  An approximately unbiased estimate of $E_y E_x[\log(g(x|\hat{\theta}(y))]$ for **large sample** and **"good" model** is

$$\log(\mathcal{L}(\hat{\theta}|y)) - k$$

  ▼ $\mathcal{L}$: likelihood function.

  ▼ $\hat{\theta}$: maximum likelihood estimate of θ.

  ▼ k: number of estimated parameters (including the variance).

- **Remark**

  ▼ *"Good" model*: the model that is close to f in the sense of having a small K-L value.

- **Maximum Likelihood Case**

$$AIC = \underbrace{-2\log \mathcal{L}(\hat{\theta}|y)}_{\textbf{bias}} + \underbrace{2k}_{\textbf{variance}}$$

  - ▼ Calculate AIC value for each model with the **same data set**, and the "best" model is the one with minimum AIC value.
  - ▼ The value of AIC depends on data y, which leads to model selection uncertainty.

- **Least-Squares Case**

  Assumption: i.i.d. normally distributed errors

$$AIC = n\log\left(\frac{RSS}{n}\right) + 2k$$

  - ▼ RSS is estimated residual of fitted model.

Takeuchi's Information Criterion (1976)

useful in cases where the model is not particular close to truth.

- **Model Selection Criterion**

$$\underset{g \in G}{\text{Maximizing}}\ E_y E_x[\log(g(x|\hat{\theta}(y)))]$$

- **Key Result**

  An approximately unbiased estimator of $E_y E_x[\log(g(x|\hat{\theta}(y)]$ for **large sample** is

$$\log(\mathcal{L}(\hat{\theta}|y)) - \mathrm{tr}(J(\theta_0)I(\theta_0)^{-1})$$

  ▼ $J(\theta_0) = E_f\left[\left(\frac{\partial}{\partial\theta}\log(g(x|\theta))\right)\left(\frac{\partial}{\partial\theta}\log(g(x|\theta))\right)^T\right]_{|\theta=\theta_0}$

  ▼ $I(\theta_0) = E_f\left[-\frac{\partial^2 \log(g(x|\theta))}{\partial\theta_i\theta_j}\right]_{|\theta=\theta_0}$

- **Remark**

  ▼ If $g \equiv f$, then $I(\theta_0) = J(\theta_0)$. Hence $\mathrm{tr}(J(\theta_0)I(\theta_0)^{-1}) = k$.

  ▼ If g is close to f, then $\mathrm{tr}(J(\theta_0)I(\theta_0)^{-1}) \approx k$.

- **TIC**

$$TIC = -2\log(\mathcal{L}(\hat{\theta}|y)) + 2\mathrm{tr}(\widehat{J}(\hat{\theta})[\widehat{I}(\hat{\theta})]^{-1}),$$

where $\widehat{I}(\hat{\theta})$ and $\widehat{J}(\hat{\theta})$ are both $k \times k$ matrix, and

$$\widehat{I}(\hat{\theta}) = -\frac{\partial^2 \log(g(x|\hat{\theta}))}{\partial\theta^2} \quad \longrightarrow \text{ estimate of } I(\theta_0)$$

$$\widehat{J}(\hat{\theta}) = \sum_{i=1}^{n} \left[\frac{\partial}{\partial\theta}\log(g(x_i|\hat{\theta}))\right] \left[\frac{\partial}{\partial\theta}\log(g(x_i|\hat{\theta}))\right]^T \quad \longrightarrow \text{ estimate of } J(\theta_0)$$

- **Remark**
  - ▼ Attractive in theory.
  - ▼ Rarely used in practice because we need a very large sample size to obtain good estimates for both $I(\theta_0)$ and $J(\theta_0)$.

A Small Sample AIC

use in the case where the sample size is small relative to the number of parameters
rule of thumb: $n/k < 40$

- **Univariate Case**

  Assumption: i.i.d normal error distribution with the truth contained in the model set.

$$AIC_c = AIC + \underbrace{\frac{2k(k+1)}{n-k-1}}_{\text{bias-correction}}$$

- **Remark**

  - The bias-correction term varies by type of model (e.g., normal, exponential, Poisson).
  - In practice, AIC_c is generally suitable unless the underlying probability distribution is extremely nonnormal, especially in terms of being strongly skewed.

- **Multivariate Case**

  Assumption: each row of ϵ is i.i.d $\mathbf{N}(0, \Sigma)$.

$$AIC_c = AIC + 2\frac{k(\tilde{k} + 1 + p)}{n - \tilde{k} - 1 - p}$$

  ▼ Applying to the multivariate case:

$$Y = TB + \epsilon, \text{ where } Y \in \mathbb{R}^{n \times p}, T \in \mathbb{R}^{n \times \tilde{k}}, B \in \mathbb{R}^{\tilde{k} \times p}.$$

  ▼ p: total number of components.

  ▼ n: number of independent multivariate observations, each with p nonindependent components.

  ▼ k: total number of unknown parameters and $k = \tilde{k}p + p(p+1)/2$.

- **Remark**

  ▼ Bedrick and Tsai in [1] claimed that this result can be extended to the multivariate nonlinear regression model.

AIC Differences, Likelihood of a Model, Akaike Weights

- **AIC differences**

  Information loss when fitted model is used rather than the best approximating model

  $$\Delta_i = AIC_i - AIC_{\min}$$

  ▼ $AIC_{\min}$: AIC values for the best model in the set.

- **Likelihood of a Model**

  Useful in making inference concerning the relative strength of evidence for each of the models in the set

  $$\mathcal{L}(g_i|y) \propto \exp\left(-\frac{1}{2}\Delta_i\right), \text{ where } \propto \text{ means "is proportional to".}$$

- **Akaike Weights**

  "Weight of evidence" in favor of model i being the best approximating model in the set

  $$w_i = \frac{\exp(-\frac{1}{2}\Delta_i)}{\sum_{r=1}^{R}\exp(-\frac{1}{2}\Delta_r)}$$

Confidence Set for K-L Best Model

- **Three Heuristic Approaches (see [4])**

  - **Based on the Akaike weights w_i**

    To obtain a 95% confidence set on the actual K-L best model, summing the Akaike weights from largest to smallest until that sum is just ≥ 0.95, and the corresponding subset of models is the confidence set on the K-L best model.

  - **Based on AIC difference Δ_i**

    - $0 \leq \Delta_i \leq 2$, substantial support,
    - $4 \leq \Delta_i \leq 7$, considerable less support,
    - $\Delta_i > 10$, essentially no support.

    Remark

    - Particularly useful for nested models, may break down when the model set is large.
    - The guideline values may be somewhat larger for nonnested models.

  - **Motivated by likelihood-based inference**

    The confidence set of models is all models for which the ratio

$$\frac{\mathcal{L}(g_i|y)}{\mathcal{L}(g_{\min}|y)} > \alpha, \text{ where } \alpha \text{ might be chosen as } \frac{1}{8}.$$

Multimodel Inference

- **Unconditional Variance Estimator**

$$\widehat{\mathrm{var}}(\hat{\bar{\theta}}) = \left[\sum_{i=1}^{R} w_i \sqrt{\widehat{\mathrm{var}}(\hat{\theta}_i|g_i) + (\hat{\theta}_i - \hat{\bar{\theta}})^2}\right]^2$$

  - ▼ θ is a parameter in common to all R models.
  - ▼ $\hat{\theta}_i$ means that the parameter θ is estimated based on model g_i,
  - ▼ $\hat{\bar{\theta}}$ is a model-averaged estimate $\hat{\bar{\theta}} = \sum_{i=1}^{R} w_i \hat{\theta}_i$.

- **Remark**

  - ▼ "Unconditional" means not conditional on any particular model, but still conditional on the full set of models considered.
  - ▼ If θ is a parameter in common to only a subset of the R models, then w_i must be recalculated based on just these models (thus these new weights must satisfy $\sum w_i = 1$).
  - ▼ Use unconditional variance unless the selected model is strongly supported (for example, $w_{\min} > 0.9$).

Summary of Akaike Information Criteria

- **Advantages**
  - Valid for both nested and nonnested models.
  - Compare models with different error distribution.
  - Avoid multiple testing issues.
- **Selected Model**
  - The model with minimum AIC value.
  - Specific to given data set.
- **Pitfall in Using Akaike Information Criteria**
  - **Can not be used to compare models of different data sets.**

    For example, if nonlinear regression model g_1 is fitted to a data set with $n = 140$ observations, one cannot validly compare it with model g_2 when 7 outliers have been deleted, leaving only $n = 133$.

- **Should use the same response variables for all the candidate models.**

  For example, if there was interest in the normal and log-normal model forms, the models would have to be expressed, respectively, as

$$g_1(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right],\ g_2(x|\mu,\sigma) = \frac{1}{x\sqrt{2\pi}\sigma}\exp\left[-\frac{(\log(x)-\mu)^2}{2\sigma^2}\right],$$

  instead of

$$g_1(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right],\ g_2(\log(x)|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{(\log(x)-\mu)^2}{2\sigma^2}\right].$$

- **Do not mix null hypothesis testing with information criterion.**
  - Information criterion is not a "test", so avoid use of "significant" and "not significant", or "rejected" and "not rejected" in reporting results.
  - Do not use AIC to rank models in the set and then test whether the best model is "significantly better" than the second-best model.
- **Should retain all the components of each likelihood in comparing different probability distributions.**

References

[1] E.J. Bedrick and C.L. Tsai, Model Selection for Multivariate Regression in Small Samples, *Biometrics*, 50 (1994), 226–231.

[2] H. Bozdogan, Model Selection and Akaike's Information Criterion (AIC): The General Theory and Its Analytical Extensions, *Psychometrika*, 52 (1987), 345–370.

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[4] K.P. Burnham and D.R. Anderson, *Model Selection and Inference: A Practical Information-Theoretical Approach*, (1998), New York: Springer-Verlag.

[5] K.P. Burnham and D.R. Anderson, Multimodel Inference: Understanding AIC and BIC in Model Selection, *Sociological methods and research*, 33 (2004), 261–304.

[6] C.M. Hurvich and C.L. Tsai, Regression and Time Series Model Selection in Small Samples, *Biometrika*, 76 (1989).