Bayesian Model Selection: Marginal Likelihood, Cross-Validation & Co

Andreas Kirsch
University of Oxford–2023

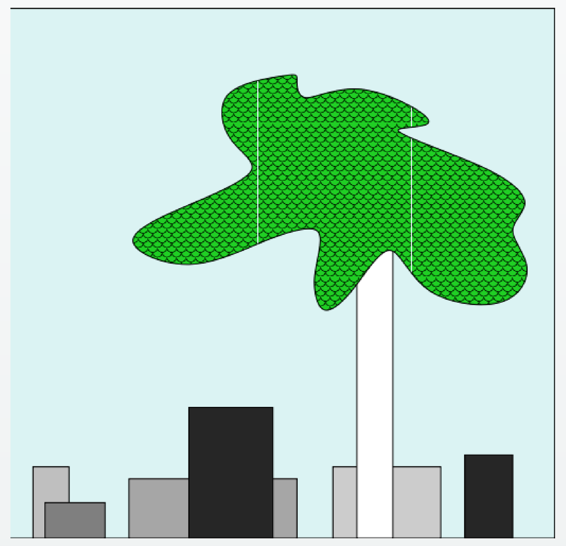
Occam's Razor

Occam's Razor is the principle that, all else being equal, the simplest explanation tends to be the right one.

Occam's Razor ↔ Bayesian Model Selection

Both minimize information/maximize likelihoods **BUT** are ambiguous about multiple data points & objectives.

Examples (left: Reddit, right: MacKay (2003))



How many objects are occluded?

Shannon's Information Content

The *information content* (or *surprisal*) of an event x with probability $\mathrm{p}(x)$ is:

$$\mathrm{H}[x] = -\log \mathrm{p}(x) \tag{1}$$

Likewise, the *entropy* of a random variable $\boldsymbol{X}$ is:

$$\mathrm{H}[\boldsymbol{X}] = \mathbb{E}_{\mathrm{p}(\boldsymbol{X})}\,[\mathrm{H}[\boldsymbol{X}]] = -\mathbb{E}_{\mathrm{p}(\boldsymbol{X})}\,[\log \mathrm{p}(\boldsymbol{X})] \tag{2}$$

Minimum Description Length (MDL)/MLE/MAP

The **Minimum Description Length (MDL)** formalizes Occam's razor by selecting the model that minimizes the sum of the model's description length (complexity) and the data's description length given the model (fit). For a model $\boldsymbol{\phi}$ and data $(\boldsymbol{x}_n)_{n=1}^N$, the MDL criterion is:

$$\mathrm{H}[\boldsymbol{\phi}] + \mathrm{H}[(\boldsymbol{x}_n)_{n=1}^N \mid \boldsymbol{\phi}] \tag{3}$$

where $\mathrm{H}[\boldsymbol{\phi}]$ is the model's description length and $\mathrm{H}[(\boldsymbol{x}_n)_{n=1}^N \mid \boldsymbol{\phi}]$ is the data's description length given the model. The model with the lowest MDL score is selected.

Multiple vs Individual Points

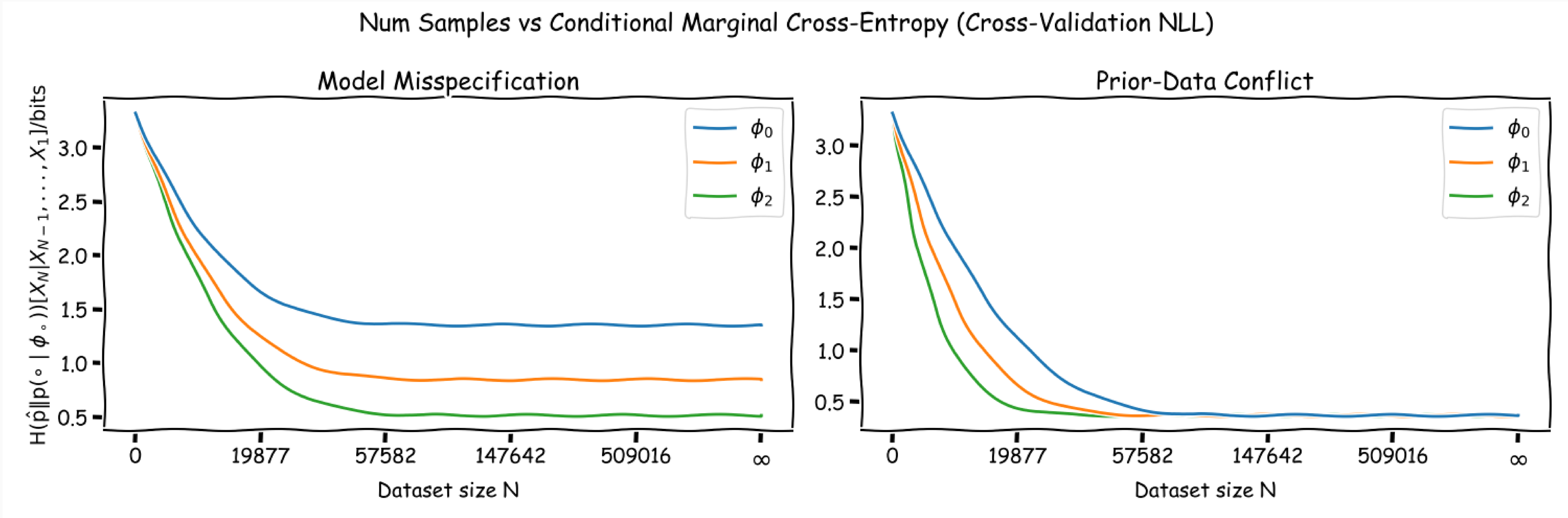
For multiple samples (given datasets), information-theoretic quantities for model selection can be computed in different ways, **leading to ambiguity**:

- **Joint Quantities** (e.g., joint marginal cross-entropy, conditional joint marginal information) substitute the dataset directly, e.g. $\mathrm{H}[\mathcal{D} \mid \boldsymbol{\phi}]$, and include **in-context learning**.
- **Individual Quantities** (e.g., marginal cross-entropy, conditional marginal cross-entropy) focus on model performance over individual points, e.g., $\mathrm{H}_{\hat{\mathrm{p}}_{\mathrm{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\boldsymbol{X}]$, similar to validation/test performance.

Different Data Regimes, Model Misspecification and Prior-Data Conflict

TL;DR

1. In the **large-data regime** (or infinite data limit), the (rate of the) joint quantities and individual quantities converge to the same values. Different models perform differently due to different levels of **model misspecification**.
2. In the **low-data regime** (and *low* can still be a lot), these quantities will not have converged, and different models can perform differently due to **model misspecification** and **prior data conflict**, which can even be *anti-correlated.*



Model misspecification occurs when the assumed model class does not contain the true data-generating process:

- Different models have different levels of misspecification.
- In the infinite data limit, the model with the lowest misspecification (i.e., the closest to the true data-generating process) will perform best.

Prior-data conflict arises when the assumed prior distribution is inconsistent with the observed data. In this scenario:

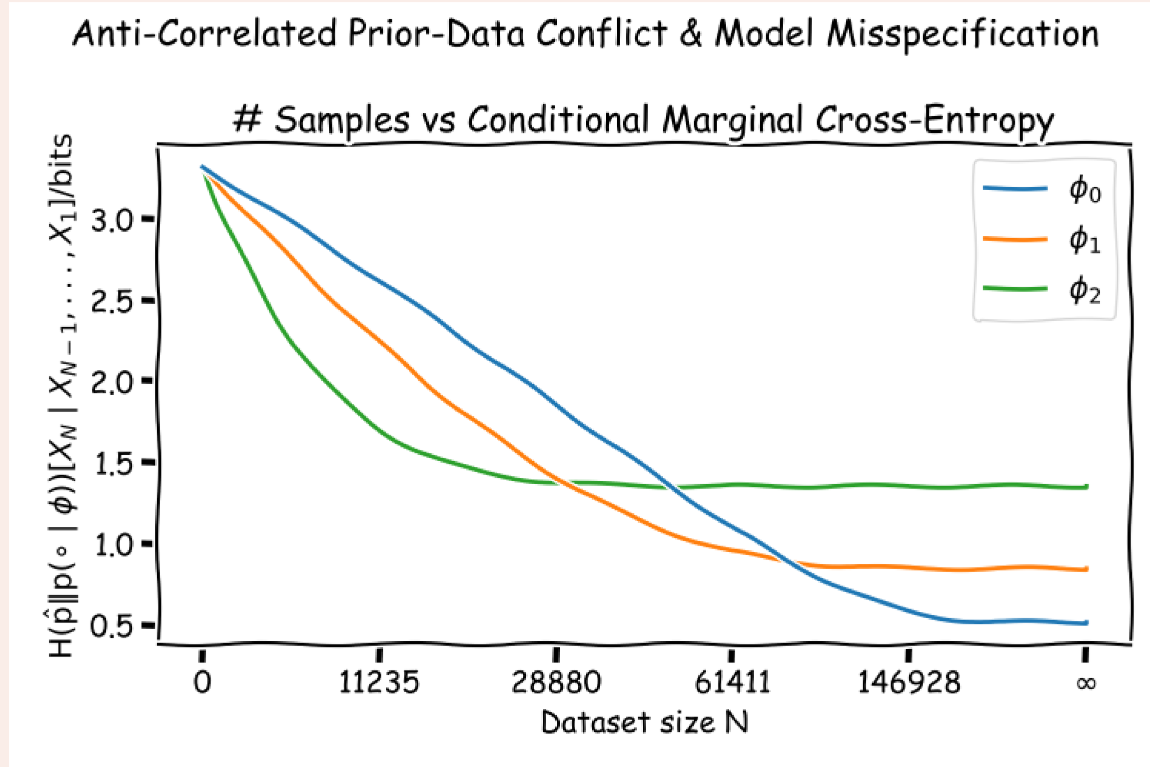
- Models with priors that are more consistent with the observed data will perform better initially.
- The effect of prior-data conflict diminishes as the dataset size increases and the likelihood term dominates the prior term.

Different Information Quantities for Model Selection

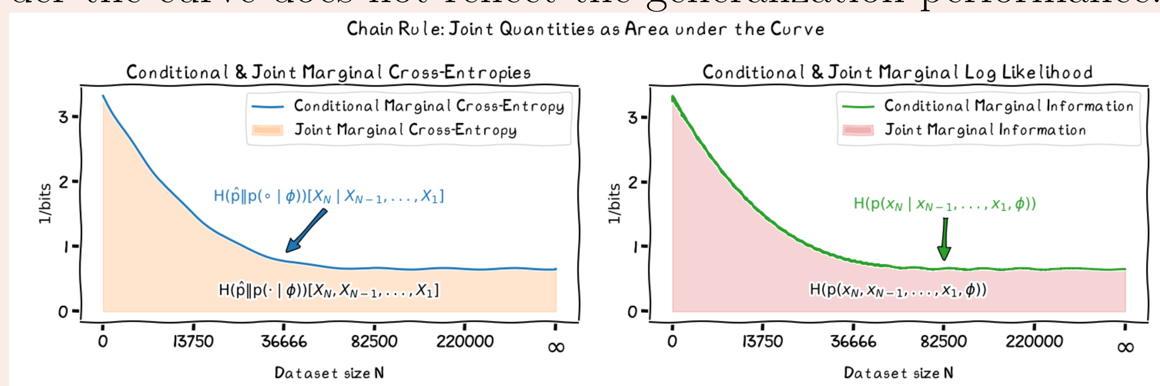
For a dataset $(\boldsymbol{x}_n)_{n=1}^N = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, we consider the following information-theoretic quantities for model selection:

- **Joint Marginal Cross-Entropy**: $\mathrm{H}_{\hat{\mathrm{p}}_{\mathrm{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\{\boldsymbol{X}_n\}_{n=1}^N]$. The expected joint information content of a dataset $(\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n)$ under the model's joint prior predictive distribution, averaged over the true data distribution. Equivalent to the **log marginal likelihood (LML)**.
- **Conditional Marginal Cross-Entropy**: $\mathrm{H}_{\hat{\mathrm{p}}_{\mathrm{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\boldsymbol{X}_n \mid \boldsymbol{X}_{n-1}, \ldots, \boldsymbol{X}_1]$. The expected information content of a single data point $\boldsymbol{X}_n$ conditioned on the previous data points $(\boldsymbol{X}_{n-1}, \ldots, \boldsymbol{X}_1)$ under the model's predictive distribution, averaged over the true data distribution. Equivalent to **leave-one-out cross-validation**.
- **Conditional Joint Marginal Information**: $\mathrm{H}[\{\boldsymbol{x}_n\}_{n=N-k+1}^N \mid \{\boldsymbol{x}_n\}_{n=1}^{N-k}, \boldsymbol{\phi}]$. The joint information content of a dataset $\{\boldsymbol{x}_n\}_{n=N-k+1}^N$ conditioned on a previous dataset $\{\boldsymbol{x}_n\}_{n=1}^{N-k}$ under the model's joint predictive distribution. This is data-order dependent. Also known as the (negative) **conditional log marginal likelihood (CLML)** (Lotfi et al., 2022, main paper).
- **Conditional Joint Marginal Cross-Entropy**: $\mathrm{H}_{\hat{\mathrm{p}}_{\mathrm{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\{\boldsymbol{X}_n\}_{n=N-k+1}^N \mid \{\boldsymbol{X}_n\}_{n=1}^{N-k}]$. The expected joint information content of a dataset $\{\boldsymbol{X}_n\}_{n=N-k+1}^N$ conditioned on a previous dataset $\{\boldsymbol{X}_n\}_{n=1}^{N-k}$ under the model's joint predictive distribution, averaged over the true data distribution. Measures the model's online learning (or in-context learning) performance. Also known as the (negative) **conditional log marginal likelihood (CLML)** (Lotfi et al., 2022, appendix).

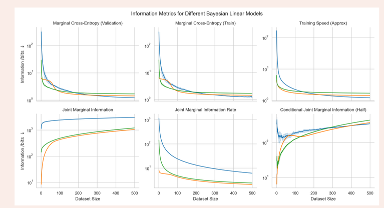
Failures & Prior Art



With anti-correlated prior-data conflict and model misspecification, existing methods fail: Training speed methods (TSE, TSE-E, TSE-EMA) (Lyle et al., 2020; Ru et al., 2021) and the conditional log marginal likelihood (CLML) (Fong and Holmes, 2020; Lotfi et al., 2022) *essentially* approximate the generalization loss by averaging under the loss curve might and might prefer models that generalize worse in the low-data regime when the (partial) area under the curve does not reflect the generalization performance.



The different metrics from prior art can fail when model misspecification and prior-data conflict are anti-correlated. Here, for a simple binary regression task:



Details

References

Fong, E. and Holmes, C. C. (2020). On the marginal likelihood and cross-validation. *Biometrika*, 107(2):489–496.

Lotfi, S., Izmailov, P., Benton, G., Goldblum, M., and Wilson, A. G. (2022). Bayesian model selection, the marginal likelihood, and generalization. In *International Conference on Machine Learning*, pages 14223–14247. PMLR.

Lyle, C., Schut, L., Ru, R., Gal, Y., and van der Wilk, M. (2020). A bayesian perspective on training speed and model selection. *Advances in neural information processing systems*, 33:10396–10408.

MacKay, D. J. (2003). *Information theory, inference and learning algorithms*. Cambridge university press.

Ru, B., Lyle, C., Schut, L., Fil, M., van der Wilk, M., and Gal, Y. (2021). Speedy performance estimation for neural architecture search. In Beygelzimer, A., Dauphin, Y., Liang, P., and Vaughan, J. W., editors, *Advances in Neural Information Processing Systems*.

LaTeX TikZposter