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

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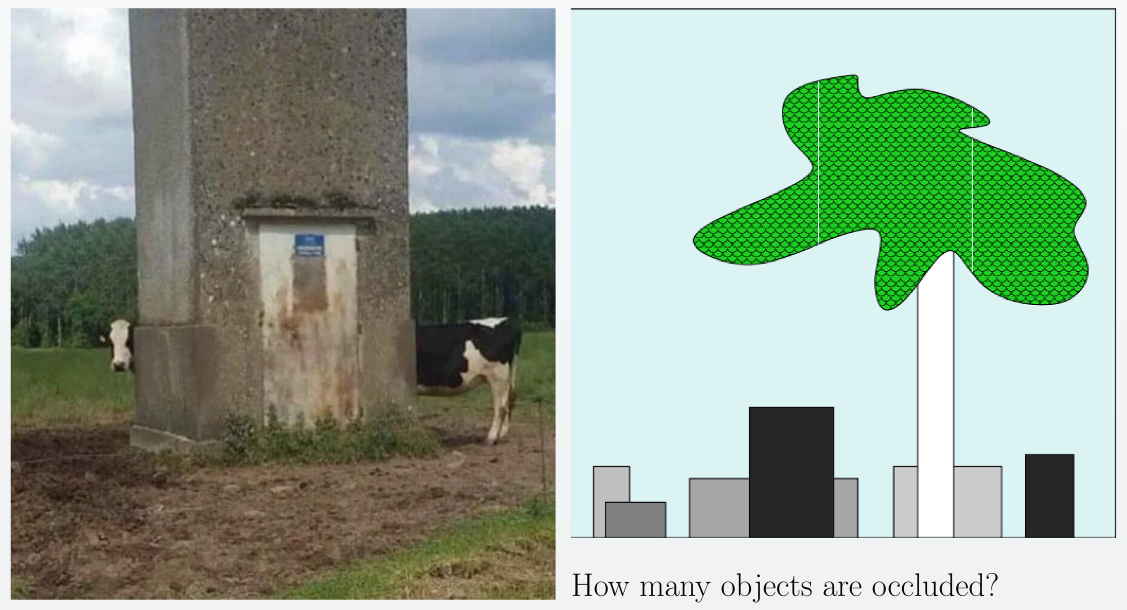
Occam's Razor

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:

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

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

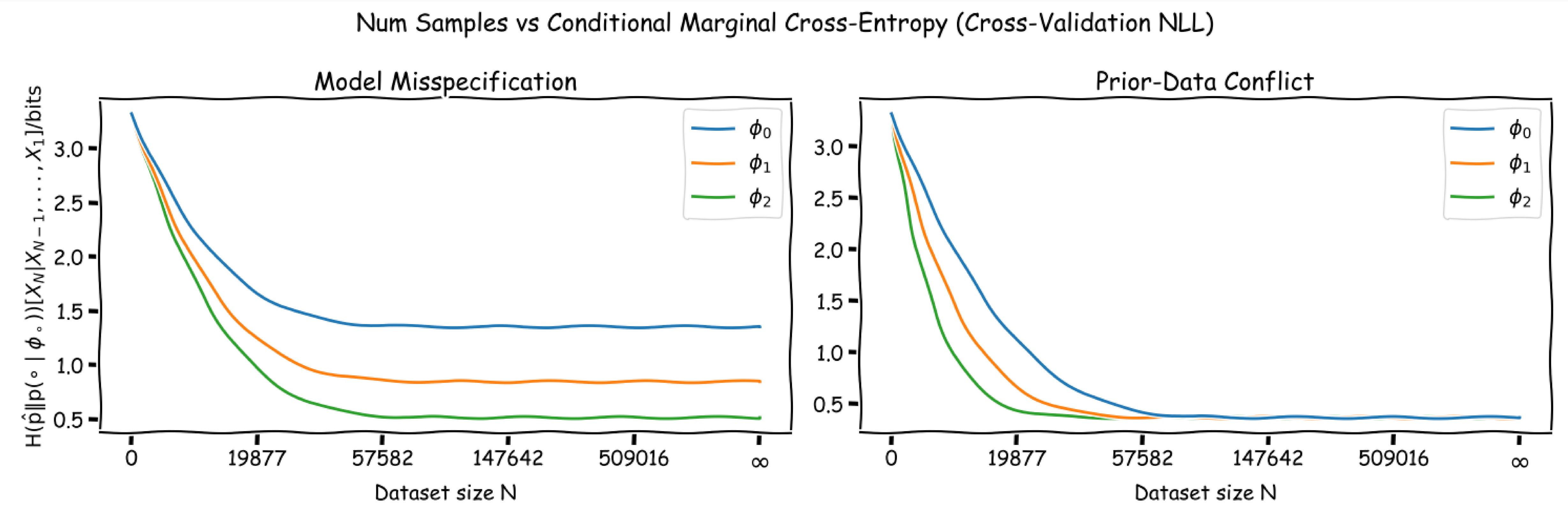
For multiple samples (given datasets), information-theoretic quantities for model selection can be computed in different ways, **leading to ambiguity**:

- **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., $\mathrm{H}_{\hat{\mathrm{p}}_{\text{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\boldsymbol{X}]$, 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 not aligned with the observed data. In this scenario:

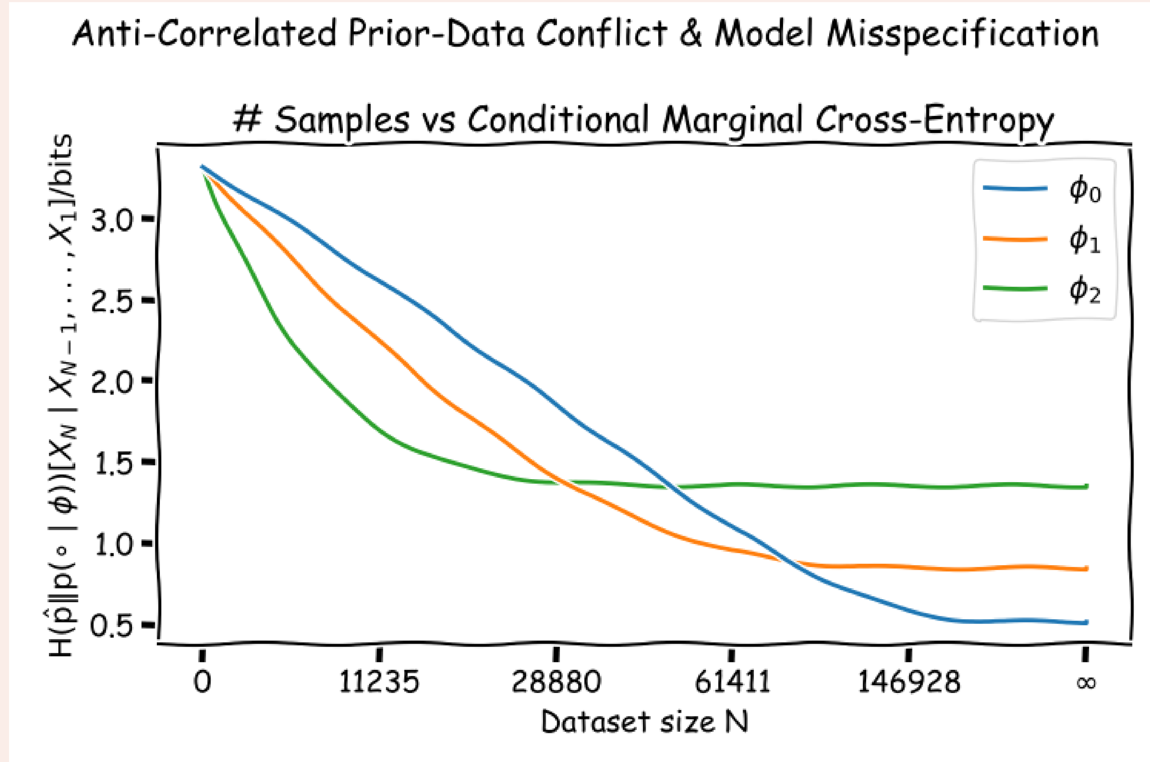
- Models with priors that are less aligned with the observed data will perform worse initially.
- The effect of prior-data conflict diminishes as the dataset size increases and the likelihood term dominates the prior term.

Different Information Quantities for Model Selection

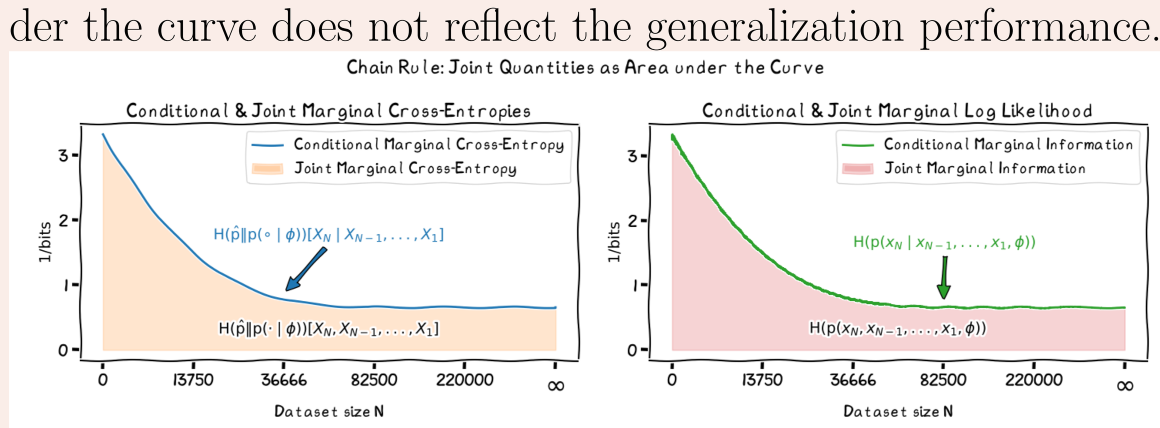
For a dataset $(\boldsymbol{x}_n)_{n=1}^N = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, we consider the following information-theoretic quantities for model selection:

- **Joint Marginal Cross-Entropy**: $\mathrm{H}_{\hat{\mathrm{p}}_{\text{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\{\boldsymbol{X}_n\}_{n=1}^N]$. 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**: $\mathrm{H}_{\hat{\mathrm{p}}_{\text{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\boldsymbol{X}_n \mid \boldsymbol{X}_{n-1}, \ldots, \boldsymbol{X}_1]$. 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**: $\mathrm{H}_{\hat{\mathrm{p}}_{\text{data}} \| \mathrm{p}(\cdot \mid \boldsymbol{\phi})}[\{\boldsymbol{X}_n\}_{n=N-k+1}^N \mid \{\boldsymbol{X}_n\}_{n=1}^{N-k}]$. 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).

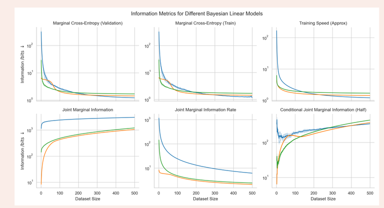
Failures & Prior Art



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

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