Computational Cognitive Science

Lecture 7: Model comparison and selection

Chris Lucas

School of Informatics

University of Edinburgh

October 11, 2022

Readings

- Chapter 10 of F&L
- "Ockham's razor and Bayesian Analysis" (link)

Recommended:

• "A note on the evidence and Bayesian Occam's razor" (link)

Model comparison

We have discussed estimating parameters conditional on a model.

- That may be all we need, if we can capture different theories as parameter choices in a single model
- In practice, we may want to compare qualitatively different models

How do we choose between models?

Criteria for choosing models

We prefer models that are

- Predictively useful
- Compatible with our data
- Likely to be correct, or closer to a correct model

(Understandable, too)

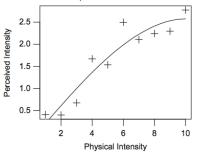
Two models of perceived intensity

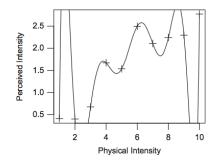
- M₁: Perceived intensity is a 2nd order polynomial function of physical intensity
- M₂: Perceived intensity is a **9th** order polynomial function of physical intensity

(Ignore the fact that we could distinguish between these models w/a single model and suitable priors over parameters)

Two models of perceived intensity

Both models, with MLE fits¹:





Which is better?

¹Figure 10.1 in F&L.

Two models

- Is the complex polynomial going to give good predictions?
 - $p(y_{K+1}|\mathbf{y}, \mathcal{M}_2)$
- Is the complex polynomial compatible with our data?
 - $p(\mathbf{y}|\mathcal{M}_2)$
- Is the complex polynomial the right generative model??
 - $p(\mathcal{M}_2|\mathbf{y})$

An important distinction:

- A specific 9th order polynomial, versus
- **some** 9th order polynomial.

Predictive accuracy

- Is the complex polynomial going to give good predictions?
 - $p(y_{K+1}|\mathbf{y},\mathcal{M}_2)$

Suppose we have a model where all we care about is RMSE, and we can only obtain point-estimate predictions.

Are there any principles that should guide how we define a model?

Geman et al.² described *bias-variance dilemma*, explaining why "tabula rasa" models are not desirable.

²"Neural networks and the bias-variance dilemma" (1992) by Geman, Bienentock, and Doursat.

Bias and variance

- The expected RMSE of a regression model can be decomposed:
 - Error due to bias: The difference between the expected predictions of the model (under all possible data) and the real mean
 - Error due to *variance*: How much the model's predictions vary as a function of the specific data it has been given

Bias and variance

- The ideal model:
 - predictions are matched to reality (in expectation); no bias-based error
 - predictions don't depend on idiosyncrasies of data; no variance-based error
 - Extreme version: A perfectly confident and accurate prior
- Highly flexible models will do poorly unless large data sets are available

The lesson: If we have a priori information or constraints, we should use them!

Two models

For probababilistic models, predictive accuracy relates to other desiderata:

- Is the complex polynomial compatible with our data?
 - $p(\mathbf{y}|\mathcal{M}_2)$
- Is the complex polynomial the right generative model?
 - $p(\mathcal{M}_2|\mathbf{y}) \propto p(\mathbf{y}|\mathcal{M}_2)P(\mathcal{M}_2)$

To answer these questions, we need the *marginal likelihood* of our data.

Two models

Marginal likelihood:

$$p(\mathbf{y}|\mathcal{M}) = \int_{\boldsymbol{\theta}} p(\mathbf{y}|\mathcal{M}, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{M}) d\boldsymbol{\theta}$$

 $\neq p(\mathbf{y}|\mathcal{M}, \hat{\boldsymbol{\theta}})$

- Flexible models can accommodate a wide variety of patterns
- If those patterns are not present in our data, they're bad models

Flexibility and overfitting: Likelihood

What if we specify $p(\theta)$ at the start, and compute $p(\mathbf{y}|\mathcal{M})$?

That's an excellent solution, when it's viable.

However:

- We must choose priors carefully
- ullet Integrating over $oldsymbol{ heta}$ is often expensive or impossible

Model comparison without marginal likelihood

What if we can't compute the marginal likelihood, but can compute likelihoods and MLEs?

• Compare predictive accuracy/likelihood on held-out test data

Model comparison without marginal likelihood

What if we don't have a test set?

- E.g., using a data set where alternative models were fitted to the whole set
- Very few data points, s.t., estimating parameters already difficult

Three common approaches:

- **1** Likelihood ratios vs χ^2
- AIC and BIC
- Cross-validation

Nested models and χ^2

Suppose \mathcal{M}_1 is a special case of \mathcal{M}_2 ; \mathcal{M}_2 has additional parameters and reduces to \mathcal{M}_1 for specific values of these parameters. We can say \mathcal{M}_1 is *nested* in \mathcal{M}_2 .

Even if the additional parameters of \mathcal{M}_2 are useless – they just allow it to fit noise – the negative log likelihood will be slightly lower.

Nested models and likelihood ratios

However, under certain assumptions and as n goes to infinity, that improvement (times 2) will converge to a χ^2 distribution with df equal to the difference in dimensionality³.

As a result, one can compare the difference in MLE likelihoods to a χ^2 distribution to support or reject the hypothesis that the complex model is no better.

$$2 \cdot [\log(p(\mathbf{y}|\hat{\boldsymbol{\theta}_2}, \mathcal{M}_2) - \log(p(\mathbf{y}|\hat{\boldsymbol{\theta}_1}, \mathcal{M}_1))]$$

Caveats:

- If models are nested, there are often nice Bayesian approaches
- Null hypothesis significance test

³To learn more, see Wilks' theorem (link)

AIC

Another approach: "How different is the distribution implied by my model from the real-world distribution of human behavior?"

How can we quantify this difference?

Kullback-Leibler divergence⁴:

$$\int_{\mathbf{y}} R(\mathbf{y}) \log \frac{R(\mathbf{y})}{p_M(\mathbf{y})} d\mathbf{y}$$

If these distributions are identical, divergence is zero. If the model assigns zero probability density to events that are possible, it's ∞ .

⁴Wikipedia article. Don't call it a distance.

AIC

AIC approximates relative KL divergences of models to target distribution (e.g., relative probabilities of behaviors):

$$AIC = 2k - 2 \cdot \log(p(\mathbf{y}|\boldsymbol{\theta}_{MLE}))$$

- Asymptotically agrees with leave-one-out cross-validation
- There are many alternatives, but AIC is simple and popular

AIC

Caveats:

- Approximates hold-one-out cross-validation, not extrapolation
- Approximation is asymptotic; not necessarily great for small data sets
- Parameter counting is sometime a poor way to evaluate complexity; see text
- Cross-validation makes fewer assumptions, is intuitive and robust – generally better
- ullet Consider alternatives like ${
 m AIC}_{\mathcal C}$



The best way to assess a model's predictive accuracy: Predict with it.

Prediction (again)

The best way to assess a model's predictive accuracy: Predict with it.

- Sequester a subset of your data. Don't touch it. Don't look at it. Pretend it doesn't exist.
 - To see if a model can predict the judgments or behavior of new participants or in new conditions, hold out participants and/or conditions
 - Likewise for future judgments given past judgments

Prediction (again)

The best way to assess a model's predictive accuracy: Predict with it.

- Fit models on separate data, compare their predictive log likelihoods on the sequestered data
 - No need to penalize model complexity

Cross-validation

If you want robust and efficient estimates of predictive accuracy, you can repeat those steps for your entire data set;

- Don't look at anything before building the model
- Define an automatic policy for partitioning and fitting the model
- Repeat for K "folds" (train on K-1, evaluate on 1)
- Offers approximate predictive likelihoods for new folds

In practice, cognitive scientists rarely use fully held-out test sets.

- Tend to look at data when tuning model
- Cross-validation with seen-data is still better than testing and training on the same data

Summary

If we want to choose between models, we can do the following:

- Compare marginal likelihoods
 - Easy in concept, difficult (sometimes impossible) in practice
- Compare predictive loss with fully held-out evaluation set(s)
 - In practice, typically just one partitioning
- Ompare predictive losses w/cross-validation
 - A pragmatic approach given sparse data
 - Mitigates the worst of the "train on test" problem
 - Good partitionings require care
- AIC or likelihood-ratio test
 - Blunt instrument, but common
 - See also the AIC_C, BIC, WAIC, ...