

COMS 4721: Machine Learning for Data Science

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MODEL SELECTION

MODEL SELECTION

The model selection problem

We've seen how often model parameters need to be set in advance and discussed how this can be done using cross-validation.

Another type of model selection problem is learning model order.

Model order: The complexity of a class of models

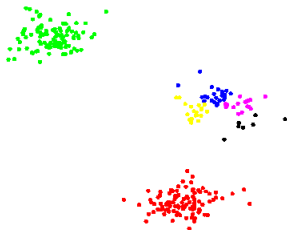
- ▶ Gaussian mixture model: How many Gaussians?
- ▶ Matrix factorization: What rank?
- ▶ Hidden Markov models: How many states?

In each of these problems, we can't simply look at the log-likelihood because a more complex model can always fit the data better.

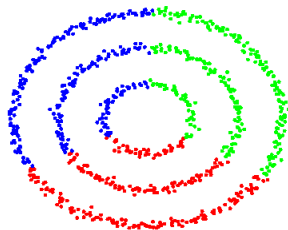
MODEL SELECTION

Model Order

We will discuss two methods for selecting an “appropriate” complexity of the model. This assumes a good model type was chosen to begin with.



(a) Inappropriate model order.



(b) Inappropriate model type.

EXAMPLE: MAXIMUM LIKELIHOOD

Notation

We write \mathcal{L} for the log-likelihood of a parameter under a model $p(x|\theta)$:

$$x_i \stackrel{iid}{\sim} p(x|\theta) \iff \mathcal{L} = \sum_{i=1}^N \log p(x_i|\theta)$$

The maximum likelihood solution is: $\theta_{\text{ML}} = \arg \max_{\theta} \mathcal{L}$.

Example: How many clusters? (wrong way)

The parameters θ could be those of a GMM. We could find θ_{ML} for different numbers of clusters and pick the one with the largest \mathcal{L} .

Problem: We can perfectly fit the data by putting each observation in its own cluster. Then shrink the variance of each Gaussian to zero.

NUMBER OF PARAMETERS

The general problem

- ▶ Models with more degrees of freedom are more prone to overfitting.
- ▶ The degrees of freedom is roughly the number of scalar parameters, K .
- ▶ By increasing K (done by increasing #clusters, rank, #states, etc.) the model can add more degrees of freedom.

Some common solutions

- ▶ **Stability:** Bootstrap sample the data, learn a model, calculate the likelihood on the original data set. Repeat and pick the best model.
- ▶ **Bayesian nonparametric methods:** Each possible value of K is assigned a prior probability. The posterior learns the best K .
- ▶ **Penalization approaches:** A penalty term makes adding parameters expensive. Must be overcome by a greater improvement in likelihood.

PENALIZING MODEL COMPLEXITY

General form

Define a *penalty function* on the number of model parameters. Instead of maximizing \mathcal{L} , minimize $-\mathcal{L}$ and add a chosen penalty.

Two popular penalties are:

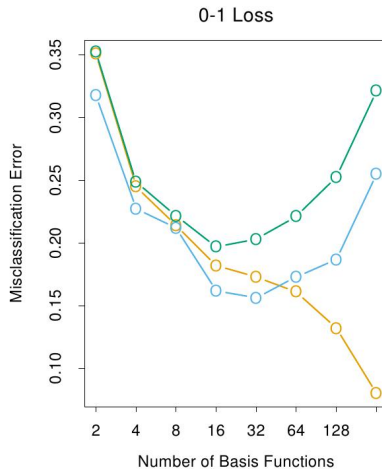
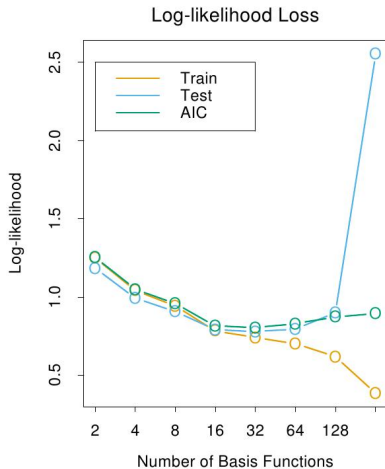
- ▶ **Akaike information criterion (AIC):** $-\mathcal{L} + K$
- ▶ **Bayesian information criterion (BIC):** $-\mathcal{L} + \frac{1}{2}K \ln N$

When $\frac{1}{2} \ln N > 1$, BIC encourages a simpler model (happens when $N \geq 8$).

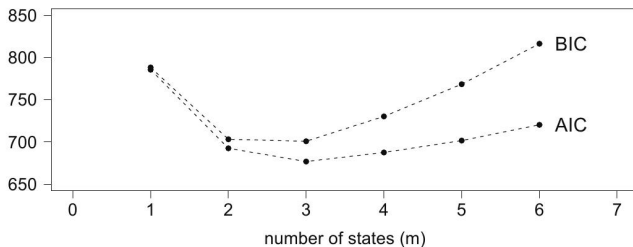
Example: For NMF with an $M_1 \times M_2$ matrix and rank R factorization,

$$\text{AIC} \rightarrow (M_1 + M_2)R, \quad \text{BIC} \rightarrow \frac{1}{2}(M_1 + M_2)R \ln(M_1 M_2)$$

EXAMPLE OF AIC OUTPUT



EXAMPLE: AIC vs BIC ON HMM



model	$-\log L$	AIC	BIC
'1-state HM'	391.9189	785.8	788.5
2-state HM	342.3183	692.6	703.3
3-state HM	329.4603	676.9	701.0
4-state HM	327.8316	687.7	730.4
5-state HM	325.9000	701.8	768.6
6-state HM	324.2270	720.5	816.7
indep. mixture (2)	360.3690	726.7	734.8
indep. mixture (3)	356.8489	723.7	737.1
indep. mixture (4)	356.7337	727.5	746.2

Notice:

- ▶ Likelihood is always improving
- ▶ Only compare location of AIC and BIC minima, not the values.

DERIVATION OF BIC

AIC AND BIC

Recall the two penalties:

- ▶ **Akaike information criterion (AIC):** $-\mathcal{L} + K$
- ▶ **Bayesian information criterion (BIC):** $-\mathcal{L} + \frac{1}{2}K \ln N$

Algorithmically, there is no extra work required:

1. Find the ML solution of the selected models and calculate $-\mathcal{L}$.
2. Add the AIC or BIC penalties to get scores and pick a model.

Q: Where do these penalties come from? Currently they seem arbitrary.

A: We will derive BIC next. AIC also has a theoretical motivation, but we will not discuss that derivation.

DERIVING THE BIC

Imagine we have r candidate models, $\mathcal{M}_1, \dots, \mathcal{M}_r$. For example, r HMMs each having a different number of states.

We also have data $\mathcal{D} = \{x_1, \dots, x_N\}$. We want the posterior of each \mathcal{M}_i .

$$p(\mathcal{M}_i|\mathcal{D}) = \frac{p(\mathcal{D}|\mathcal{M}_i)p(\mathcal{M}_i)}{\sum_j p(\mathcal{D}|\mathcal{M}_j)p(\mathcal{M}_j)}$$

If we assume a uniform prior distribution on models, then because the denominator is constant in \mathcal{M}_i , we can pick

$$\mathcal{M} = \arg \max_{\mathcal{M}_i} \ln p(\mathcal{D}|\mathcal{M}_i) = \ln \int p(\mathcal{D}|\theta, \mathcal{M}_i)p(\theta|\mathcal{M}_i)d\theta$$

By integrating out all parameters of the model, we're choosing the model with the largest *marginal likelihood* of the data. This is usually not solvable.

DERIVING THE BIC

We will see how the BIC arises from the approximation,

$$\mathcal{M} = \arg \max_{\mathcal{M}_i} \ln p(\mathcal{D}|\mathcal{M}_i) \approx \arg \max_{\mathcal{M}_i} \ln p(\mathcal{D}|\theta_{\text{ML}}, \mathcal{M}_i) - \frac{1}{2}K_i \ln N$$

Step 1: Recognize that the difficulty is with the integral

$$\ln p(\mathcal{D}|\mathcal{M}_i) = \ln \int p(\mathcal{D}|\theta)p(\theta)d\theta.$$

\mathcal{M}_i determines $p(\mathcal{D}|\theta)$ and $p(\theta)$, but not write \mathcal{M}_i for now.

Step 2: Approximate this integral using a second-order Taylor expansion.

DERIVING THE BIC

1. We want to calculate:

$$\ln p(\mathcal{D}|\mathcal{M}) = \ln \int p(\mathcal{D}|\theta)p(\theta)d\theta = \ln \int \exp\{\ln p(\mathcal{D}|\theta)\}p(\theta)d\theta$$

2. We use a second-order Taylor expansion of $\ln p(\mathcal{D}|\theta)$ at the point θ_{ML} ,

$$\begin{aligned}\ln p(\mathcal{D}|\theta) &\approx \ln p(\mathcal{D}|\theta_{\text{ML}}) + (\theta - \theta_{\text{ML}})^T \underbrace{\nabla \ln p(\mathcal{D}|\theta_{\text{ML}})}_{= 0} \\ &\quad + \frac{1}{2}(\theta - \theta_{\text{ML}})^T \underbrace{\nabla^2 \ln p(\mathcal{D}|\theta_{\text{ML}})}_{= -\mathcal{J}(\theta_{\text{ML}})}(\theta - \theta_{\text{ML}})\end{aligned}$$

3. Approximate $p(\theta)$ as uniform and plug this approximation back in,

$$\ln p(\mathcal{D}|\mathcal{M}) \approx \ln p(\mathcal{D}|\theta_{\text{ML}}) + \ln \int \exp \left\{ -\frac{1}{2}(\theta - \theta_{\text{ML}})^T \mathcal{J}(\theta_{\text{ML}})(\theta - \theta_{\text{ML}}) \right\} d\theta$$

DERIVING THE BIC

Observation: The integral is the normalizing constant of a Gaussian,

$$\int \exp \left\{ -\frac{1}{2}(\theta - \theta_{\text{ML}})^T \mathcal{J}(\theta_{\text{ML}})(\theta - \theta_{\text{ML}}) \right\} d\theta = \left(\frac{2\pi}{|\mathcal{J}(\theta_{\text{ML}})|} \right)^{K/2}$$

Remember the definition that

$$-\mathcal{J}(\theta_{\text{ML}}) = \nabla^2 \ln p(\mathcal{D}|\theta_{\text{ML}}) \stackrel{(a)}{=} N \underbrace{\sum_{i=1}^N \frac{1}{N} \nabla^2 \ln p(x_i|\theta_{\text{ML}})}_{\text{converges as } N \text{ increases}}$$

(a) is by the i.i.d. model assumption made at the beginning of the lecture.

DERIVING THE BIC

4. Plugging this in,

$$\ln p(\mathcal{D}|\mathcal{M}) \approx \ln p(\mathcal{D}|\theta_{\text{ML}}) + \frac{K}{2} \ln \left(\frac{2\pi}{|\mathcal{J}(\theta_{\text{ML}})|} \right)$$

$$\text{and } |\mathcal{J}(\theta_{\text{ML}})| = N \left| \sum_{i=1}^N \frac{1}{N} \nabla^2 \ln p(x_i|\theta_{\text{ML}}) \right|.$$

Conclusion. Therefore we arrive at the BIC,

$$\ln p(\mathcal{D}|\mathcal{M}) \approx \ln p(\mathcal{D}|\theta_{\text{ML}}) - \frac{1}{2}K \ln N + \underbrace{\text{something not growing with } N}_{O(1) \text{ term, so we ignore it}}$$

SOME NEXT STEPS

ICML SESSIONS (SUBSET)

The International Conference on Machine Learning (ICML) is one of the top ML conferences. Many of the past session titles should look familiar:

- ▶ Gaussian Processes
- ▶ PCA and Subspace Models
- ▶ Supervised Learning
- ▶ Matrix Completion and Graphs
- ▶ Clustering and Nonparametrics
- ▶ Active Learning
- ▶ Clustering
- ▶ Boosting and Ensemble Methods
- ▶ Matrix Factorization
- ▶ Kernel Methods
- ▶ Topic models
- ▶ Time Series and Sequences
- ▶ etc.

ICML SESSIONS (SUBSET)

Other sessions might not look so familiar:

- ▶ Reinforcement Learning
- ▶ Bandits
- ▶ Optimization: 13 separate sessions last year (a lot!)
- ▶ Bayesian nonparametrics
- ▶ Online learning
- ▶ Graphical Models
- ▶ Neural Networks and Deep Learning: 18 separate sessions last year (a lot!)
- ▶ Metric Learning and Feature Selection
- ▶ etc.

Bayesian methods are relevant to many sessions, as is theoretical computer science. Some relevant future courses to consider are on:

- ▶ Deep learning
- ▶ Optimization
- ▶ Bayesian methods
- ▶ Theoretical machine learning