Advanced probabilistic methods

Lecture 7: Model selection

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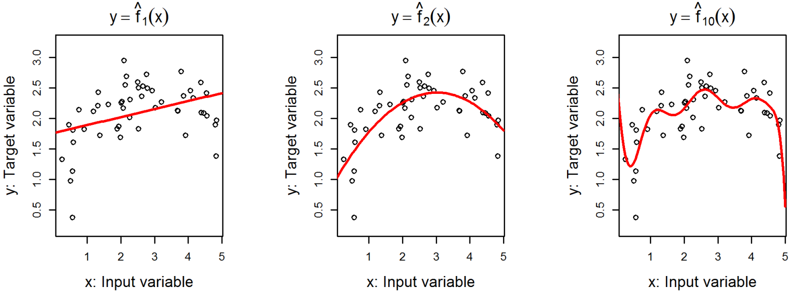
Lecture 7 overview

- Bayesian model selection
  - marginal likelihood
  - BIC, Laplace approximation
  - VB lower bound (ELBO)
- Predictive model selection
  - AIC, (DIC, WAIC, etc.)
  - Cross-validation
- Lecture based on (suggested reading):
  - Barber: Ch. 12 (Bayesian model selection)
  - *simple_elbo.pdf* (how to derive the ELBO for the simple model analytically)
  - For predictive model selection: Hastie et al. *The Elements of Statistical Learning*, (available at *http://statweb.stanford.edu/~tibs/ElemStatLearn/)*: Ch. 7.1, 7.2, 7.4, 7.5, 7.10 (for AIC and CV)

Model selection

- Possible goal may be to learn
  - **the most useful model**, for example the one that best predicts future observations
  - **the most probable model**, for example when comparing between scientific hypotheses and different hypotheses correspond to different models



Bayesian model selection

- Consider m models M_i with parameters θ_i and associated priors,

$$p(x, \theta_i | M_i) = p(x | \theta_i, M_i) p(\theta_i | M_i), \quad i \in 1, \ldots, m,$$

- We can compute the **model posterior probabilities**

$$p(M_i | x) = \frac{p(x | M_i) p(M_i)}{p(x)},$$

where

$$p(x | M_i) = \int p(x | \theta_i, M_i) p(\theta_i | M_i) d\theta_i \quad \text{and}$$

$$p(x) = \sum_{i=1}^{m} p(x | M_i) p(M_i)$$

Bayes factors

- For comparing two models, we compute the **Bayes' factor**

$$\underbrace{\frac{p(M_i|x)}{p(M_j|x)}}_{\text{Posterior odds}} = \underbrace{\frac{p(x|M_i)}{p(x|M_j)}}_{\text{Bayes' factor}} \times \underbrace{\frac{p(M_i)}{p(M_j)}}_{\text{Prior odds}},$$

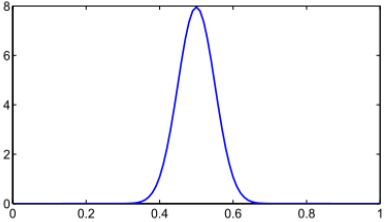
- Bayes factor is the ratio of **marginal likelihoods** $p(D|M_i)$ and it tells how much more seeing the data D has increased the probability of model M_i as opposed to model M_j.

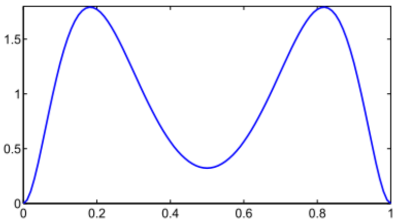
Bayes factor example (1/3)

- **Problem:** given N throws of a coin, determine whether a coin is biased or unbiased.
- Let θ denote the probability of heads. The probability of observing h heads and $N-h$ tails in a sequence of N throws is

$$p(H=h) = \binom{N}{h} \theta^h (1-\theta)^{N-h}$$

- The difference between models is encoded in the prior distribution of θ (**Left**: fair coin, **Right**: biased coin)





Bayes factor example (2/3)

- M_{fair} ('Coin is fair') corresponds to prior

$$\begin{aligned} p(\theta|M_{fair}) &= Beta(\theta|a,b) \\ &= B(a,b)^{-1}\theta^{a-1}(1-\theta)^{b-1} \end{aligned}$$

where $a = b = 50$.

- Probability of h heads in N throws of the coin is given by

$$\begin{aligned} p(x|M_{fair}) &= \int p(x|\theta, M_{fair})p(\theta|M_{fair})d\theta \\ &= \binom{N}{h} B(a,b)^{-1} \int \theta^h(1-\theta)^{N-h}\theta^{a-1}(1-\theta)^{b-1}d\theta \\ &= \binom{N}{h} B(a,b)^{-1} \int \theta^{h+a-1}(1-\theta)^{N-h+b-1}d\theta \\ &= \binom{N}{h} B(a,b)^{-1} B(h+a, N-h+b) \end{aligned}$$

Bayes factor example (3/3)

- M_{biased} ('Coin is biased') corresponds to assuming

$$p(\theta|M_2) = 0.5 \times Beta(\theta|3,10) + 0.5 \times Beta(\theta|10,3)$$

- We get

$$p(x|M_2) = \frac{1}{2}\binom{N}{h}\left\{\frac{B(h+3, N-h+10)}{B(3,10)} + \frac{B(h+10, N-h+3)}{B(10,3)}\right\}$$

- For example with $h = 50$ and $N = 70$, we get

$$BF_{fair,biased} = \frac{p(x|M_{fair})}{p(x|M_{biased})} = 0.087.$$

This indicates that if the models are *a priori* equally likely, after seeing the data, M_{biased} is about 11 times more probable than M_{fair}.

Laplace approximation for marginal likelihood*

- Laplace approximation for $p(x|M)$

$$\log p(x|M) \approx \log p(x|\widehat{\theta}, M) + \log p(\widehat{\theta}|M) + \frac{D}{2}\log(2\pi) - \frac{1}{2}\log|H_{\widehat{\theta}}|,$$

where

$$\widehat{\theta} = \arg\max_{\theta} p(x|\theta, M)p(\theta|M)$$

is the MAP estimate and $H_{\widehat{\theta}}$ is the Hessian (second derivative for univariate θ) of

$$f(\theta) = -\log\left[p(x|\theta, M)p(\theta|M)\right]$$

at $\widehat{\theta}$.

BIC approximation for marginal likelihood*

- BIC approximation[1]

$$\mathrm{BIC}(M) = \log p(x|\widehat{\theta}, M) - \frac{D}{2}\log N$$

is obtained from the Laplace approximation by assuming $p(\theta) = const$, $H \approx NI_D$, and $N \to \infty$.

- Note that we can compute the approximate Bayes factor using

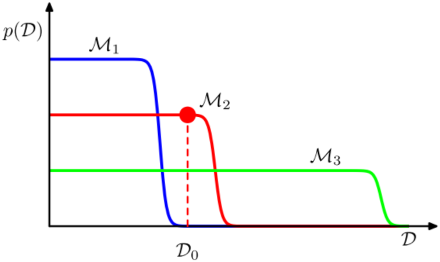
$$\mathrm{BF}_{12} = \frac{\exp(\mathrm{BIC}(M_1))}{\exp(\mathrm{BIC}(M_2))},$$

or similarly by plugging in exponentiated Laplace approximation (Laplace is better, both to be used with caution, especially with small N).

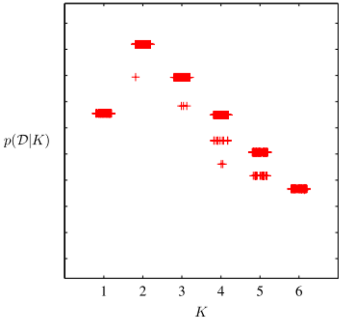
[1] Sometimes there is -2 in the front.

Bayesian model selection and Occam's razor

- When complexity of M increases, $p(x|\widehat{\theta}, M)$ always increases
- On the other hand, $p(x|M)$ **is the highest for the simplest model that can explain the data** (=Occam's razor principle)
- **Left:** illustration with model complexity increasing from M_1 to M_3
- **Right:** $p(x|K)$ for the number K of GMM components for the 'Old Faithful' data (approximated using the ELBO, see the next slides)



Bishop, Fig. 3.13



Bishop, Fig. 10.7

Variational lower bound (ELBO)

- The derivation of the VB algorithm was based on minimizing $KL(q||p)$ in
$$\log p(\mathbf{x}) = \mathcal{L}(q) + KL(q||p)$$
- When conjugate priors and exponential family distributions are used, we can compute the variational lower bound $\mathcal{L}(q)$ directly

$$\mathcal{L}(q) = \int q(\mathbf{z}) \log \left\{ \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \right\} d\mathbf{z}$$

- Computing $\mathcal{L}(q)$ gives:
  1. alternative way to define the factor updates by maximizing $\mathcal{L}(q)$.
  2. simple check of the VB algorithm - $\mathcal{L}(q)$ should never decrease.
  3. criterion to monitor convergence.
  4. an estimate of $\log p(x)$ to be used in **model selection**

Simple example: computing the ELBO

- The model:

$$p(x_n|\theta,\tau) = (1-\tau)N(x_n|0,1) + \tau N(x_n|\theta,1), \;\; n = 1,\dots,N.$$

  Prior:

$$\tau \sim Beta(\alpha_0,\alpha_0) \qquad \theta \sim N(0,\beta_0^{-1})$$

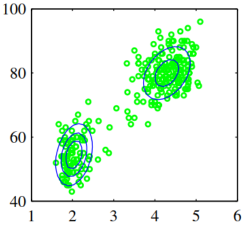
- After factorizing $\log p(\mathbf{x},\mathbf{z},\tau,\theta)$, ELBO can be written as:

$$\begin{aligned}\mathcal{L}(q) = {} & E_{q(\tau)}[\log p(\tau)] + E_{q(\theta)}[\log p(\theta)] + E_{q(\mathbf{z})q(\tau)}[\log p(\mathbf{z}|\tau)] \\ & + E_{q(\mathbf{z})q(\theta)}[\log p(\mathbf{x}|\mathbf{z},\theta)] - E_{q(\mathbf{z})}[\log q(\mathbf{z})] - E_{q(\tau)}[\log q(\tau)] \\ & - E_{q(\theta)}[\log q(\theta)].\end{aligned}$$

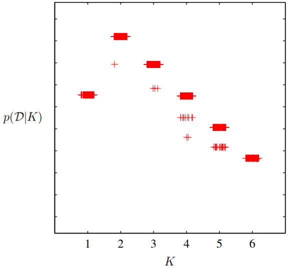
- All of the terms have analytic form (see *simple_elbo.pdf* and the next exercise).

Using the ELBO for model selection

- The ELBO $\mathcal{L}_K$ for a GMM with K components gives a lower bound of $\log p_K(x)$, where $p_K(x)$ is the marginal likelihood.
- However, VB approximates only a single mode and a GMM with K components has $K!$ equivalent modes (label switching). Hence, we add $\log(K!)$ to $\mathcal{L}_K$ when doing model selection (**right**).



Bishop, Fig. 2.21



Bishop, Fig 10.7

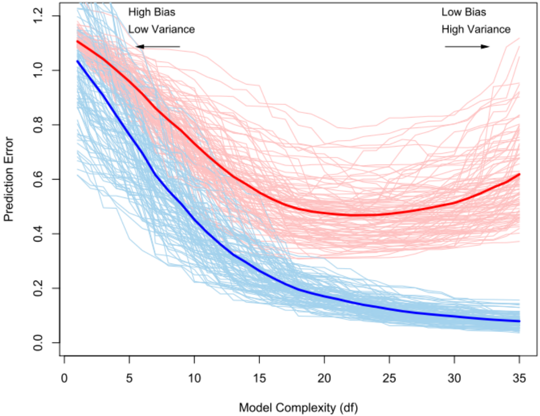
Selecting models for prediction, concepts (1/2)

- X: input variables, Y: target variable, $\widehat{f}(X)$: prediction model estimated from a training data $\mathcal{T}$.
- Loss function measures the (lack of) accuracy of prediction
- Squared loss
$$L(Y, \widehat{f}(X)) = (Y - \widehat{f}(X))^2$$
- Loss based on log-likelihood
$$L(Y, \theta(X)) = -2 \log p(Y|\theta(X)),$$
where $\theta(X)$ is a parameter of the prediction model.

Selecting models for prediction, concepts (2/2)

$$\mathrm{Err}_{\mathcal{T}} = E\left[L(Y, \widehat{f}(X))|\mathcal{T}\right] \qquad \text{(test/prediction/generalization error)}$$

$$\overline{\mathrm{err}} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \widehat{f}(x_i)) \qquad \text{(training error)}$$

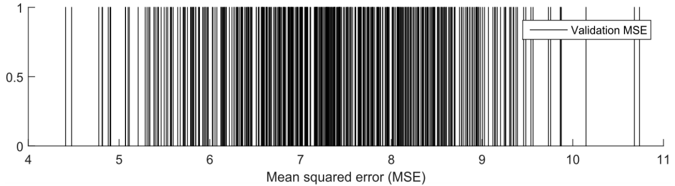


Predictive model selection criteria

- Predictive model selection criteria aim to approximate **expected prediction accuracy** in a new data set, either
  - analytically (e.g. AIC, DIC, WAIC), or
  - by efficient sample re-use (e.g. cross-validation)
- Hence, they aim to find a model that is **suitable for prediction**.
- Asymptotically, AIC and leave-one-out cross validation are equivalent.

Example (validation vs. test error)*

- Data $(\mathbf{x}_i, y_i)$ is simulated using $y_i = \sum_{i=1}^{30} w_i x_i + \epsilon_i$, where $w_i \sim U(-1,1)$, and $\epsilon_i \sim N(0, 0.1^2)$.
- 500 candidate models created by randomly selecting 10 covariates out of 30, and fitting a linear model with the selected covariates.
- $n_{Train} = 300$ and $n_{Valid} = 60$. Validation MSEs for different models:



- **Question:** What is your best guess for the test set MSE for the best model?

AIC, basic idea*

- It can be shown that for large N

$$-2 \cdot E\left[\log p(\widetilde{y}|\widehat{\theta})\right] \approx -\frac{2}{N}\log p(y|\widehat{\theta}) + 2 \cdot \frac{d}{N},$$

  where $\widetilde{y}$ is an unobserved future observation and

$$\log p(y|\widehat{\theta}) = \sum_{i=1}^{N} \log p(y_i|\widehat{\theta})$$

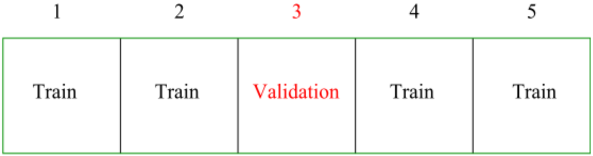
  is the log-likelihood.
- This gives rise to:

$$\text{AIC} = -\frac{2}{N}\log p(y|\widehat{\theta}) + 2 \cdot \frac{d}{N}$$

  (the smallest AIC is the best)
- **Main point**: AIC is one possible analytical approximation for the expected prediction accuracy measured using log probability of future data[2].

[2] For more Bayesian variants, see, e.g., Gelman *et al.* Stat. Comput. (2014)

Cross-Validation (CV)[3], basic idea*



- Let $\kappa : \{1, \ldots, N\} \longmapsto \{1, \ldots, K\}$ denotes the fold to which observation i belongs. Then

$$CV(\widehat{f}) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \widehat{f}^{-\kappa(i)}(x_i)),$$

  where $\widehat{f}^{-\kappa(i)}$ is the predictor model trained without fold $\kappa(i)$.
- CV yields an estimate of the expected prediction error $E\left[L(Y, \widehat{f}(X))\right]$.

[3] See, e.g., Vehtari *et al.*, *Stat. Comput.* (2017).

A wrong way to do cross-validation*

- A (wrong!) strategy for building a classifier with a large number of predictors
  1. Pre-screening of the predictors: find a subset of predictors with strong univariate correlation with the class label
  2. Using the set of predictors from pre-screening, build a multivariate classifier
  3. Use cross-validation to estimate the unknown tuning parameter and to estimate the prediction error of the final model
- **Question:** what's the problem?

The correct way*

- The correct way for building a classifier with a large number of predictors
  1. Divide the samples into K folds
  2. For each fold $k = 1, \dots, K$
     - Find a subset of predictors with strong univariate correlation with the class labels, using all samples except those in fold k.
     - Build a multivariate classifier using this set of predictors (excluding fold k)
     - Use the classifier to predict the class labels for the samples in fold k
- The class labels of the test fold should not be used at any point before predicting them in CV!

Remarks

- Bayesian model selection
  - asymptotically consistent
  - suitable when trying to find the "true" model from a set of distinct interpretable alternatives
  - heavy penalty on complexity $\rightarrow$ may produce too sparse models for prediction
  - may be sensitive to the prior on the parameters
- Predictive model selection
  - no consistency guarantees
  - no need to assume a true model
  - less penalty for model complexity $\rightarrow$ more complex models that may be suitable for prediction
- In practice people seem to use the two ways interchangeably for both goals: prediction and comparing hypotheses.

Model selection, summary

- There are two **different goals** for model selection: learning the correct model or selecting a model for prediction
- The **Bayesian model selection** gives probabilities of different models and may be more suitable if the goal is to learn the correct model.
- **Predictive model selection** criteria may be better if the goal is to use the model for prediction.
- BIC approximates Bayesian model selection, AIC and CV are related to predictive model selection.
- ELBO can be used to approximate the logarithm of the marginal likelihood $\log p_m(x)$ for model m, which can be used for Bayesian model selection.