Model Comparison

Machine Learning and Pattern Recognition

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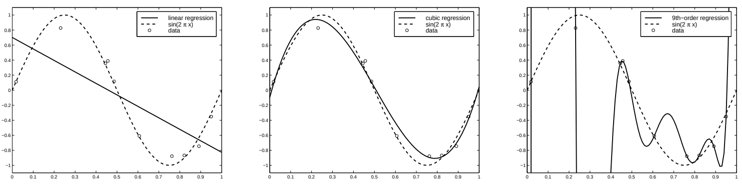
(These slides have been adapted from previous versions by Charles Sutton, Amos Storkey and David Barber

Overview

- The model selection problem
- Overfitting
- Validation set, cross validation
- Bayesian Model Comparison
- Reading: Murphy 1.4.7, 1.4.8, 6.5.3, 5.3; Barber 12.1-12.4, 13.2 up to end of 13.2.2

Model Selection

- We may entertain different models for a dataset, M_1, M_2, ..., e.g. different numbers of basis functions, different regularization parameters
- How should we choose amongst them?
- Example from supervised learning



linear cubic 9th-order

Loss and Training Error

- For input $\mathbf{x}$ the true target is $y(\mathbf{x})$ and our prediction is $f(\mathbf{x})$. The loss function

$$L(y(\mathbf{x}), f(\mathbf{x}))$$

assesses errors in prediction
- Examples
  - squared error loss $(y(\mathbf{x}) - f(\mathbf{x}))^2$,
  - 0-1 loss $I(y(\mathbf{x}), f(\mathbf{x}))$ for classification,
  - log loss $-\log p(y(\mathbf{x})|f(\mathbf{x}))$ (probabilistic predictions)
- Training error

$$E_{tr} = \frac{1}{N} \sum_{n=1}^{N} L(y(\mathbf{x}^n), f(\mathbf{x}^n))$$

- Training error consistently decreases with model complexity

Overfitting

- Generalization (or test) error

$$E_{gen} = \int L(y(\mathbf{x}), f(\mathbf{x}))\; p(\mathbf{x}, y)\; d\mathbf{x}\; dy$$

- Overfitting (Mitchell 1997, p. 67)
  A hypothesis f is said to **overfit** the data if there exists some alternative hypothesis f' such that f has a smaller training error than f', but f' has a smaller generalization error than f.

Validation Set

- Partition the available data into two: a training set (for fitting the model), and a *validation* set (aka hold-out set) for assessing performance
- *Estimate* the generalization error with

$$E_{val} = \frac{1}{V} \sum_{v=1}^{V} L(y(\mathbf{x}^v), f(\mathbf{x}^v))$$

  where we sum over cases in the validation set
- Unbiased estimator of the generalization error
- Suggested split: 70% training, 30% validation

Cross Validation

- Split the data into K pieces (folds)
- Train on $K - 1$, test on the remaining fold
- Cycle through, using each fold for testing once
- Uses all data for testing, cf. the hold-out method

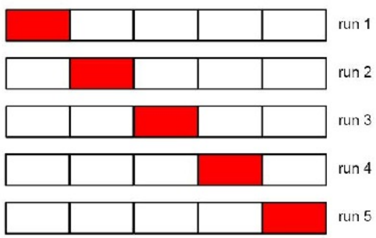


Figure credit: Murphy Fig 1.21(b)

Cross Validation: Example

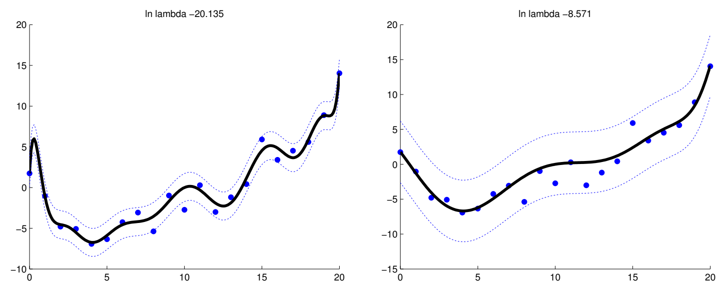


Figure credit: Murphy Fig 7.7

- Degree 14 polynomial with $N = 21$ datapoints
- Regularization term $\lambda \mathbf{w}^T \mathbf{w}$
- How to choose λ?

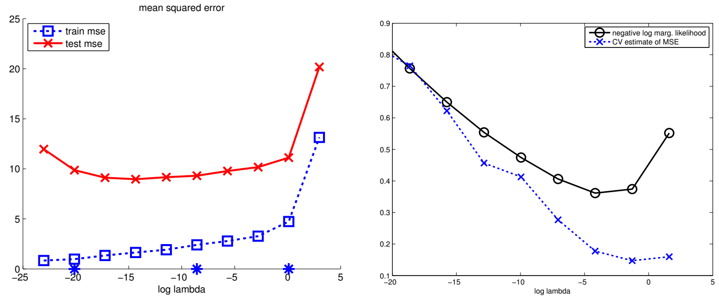


Figure credit: Murphy Fig 7.7

- Left-hand end of x-axis $\equiv$ low regularization
- Notice that training error increases monotonically with λ
- Miminum of test error is for an intermediate value of λ
- Both cross validation and a Bayesian procudure (coming soon) choose regularized models

Bayesian Model Comparison

- Have a set of different possible models

$$\mathcal{M}_i \equiv p(\mathcal{D}|\theta, M_i) \text{ and } p(\theta|M_i)$$

  for $i = 1, \ldots, K$
- Each model is set of distributions that have associated parameters. Usually some models are more complex (have more parameters) than others
- Bayesian way: Have a prior $p(M_i)$ over the set of models M_i, then compute posterior $p(M_i|\mathcal{D})$ using Bayes' rule

$$p(M_i|\mathcal{D}) = \frac{p(M_i)p(\mathcal{D}|M_i)}{\sum_{j=1}^{K} p(M_j)p(\mathcal{D}|M_j)}$$

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

  This is called the *marginal likelihood* or the *evidence*.

Comparing models

$$\text{Bayes factor} = \frac{P(\mathcal{D}|M_1)}{P(\mathcal{D}|M_2)}$$

$$\frac{P(M_1|\mathcal{D})}{P(M_2|\mathcal{D})} = \frac{P(M_1)}{P(M_2)} . \frac{P(\mathcal{D}|M_1)}{P(\mathcal{D}|M_2)}$$

$$\text{Posterior ratio} = \text{Prior ratio} \times \text{Bayes factor}$$

Strength of evidence from Bayes factor (Kass, 1995; after Jeffreys, 1961)

1 to 3	Not worth more than a bare mention
3 to 20	Positive
20 to 150	Strong
> 150	Very strong

Computing the Marginal Likelihood

- Exact for conjugate exponential models, e.g. beta-binomial, Dirichlet-multinomial, Gaussian-Gaussian (for fixed variances)
- E.g. for Dirichlet-multinomial

$$p(\mathcal{D}|M) = \frac{\Gamma(\alpha)}{\Gamma(\alpha + N)} \prod_{i=1}^{r} \frac{\Gamma(\alpha_i + N_i)}{\Gamma(\alpha_i)}$$

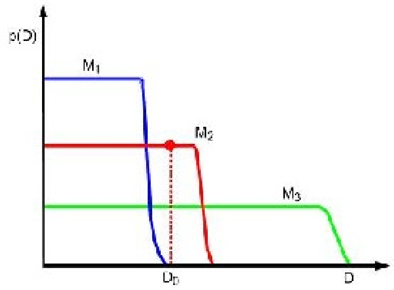
- Also exact for (generalized) linear regression (for fixed prior and noise variances)
- Otherwise various approximations (analytic and Monte Carlo) are possible

BIC approximation

$$\text{BIC} = \log p(\mathcal{D}|\hat{\theta}) - \frac{\text{dof}(\hat{\theta})}{2} \log N$$

- Bayesian information criterion (Schwarz, 1978)
- $\hat{\theta}$ is MLE
- dof($\hat{\theta}$) is the degrees of freedom in the model ($\sim$ number of parameters in the model)
- BIC penalizes ML score by a penalty term
- BIC is quite a crude approximation to the marginal likelihood

- Why Bayesian model selection? Why not compute best fit parameters and compare?
- More parameters=better fit to data. ML: bigger is better.
- But might be overfitting: only these parameters work. Many others don't.



- Prefer models that are unlikely to 'accidentally' explain the data.

Binomial Example

Example

You are an auditor of a firm. You receive details about the sales that a particular salesman is making. He attempts to make 4 sales a day to independent companies. You receive a list of the number of sales by this agent made on a number of days. Explain why you would expect the total number of sales to be binomially distributed.
If the agent was making the sales numbers up as part of a fraud, you might expect the agent (as he is a bit dim) to choose the number of sales at random from a uniform distribution.
You are aware of the fraud possibility, and you understand there is something like a 1/5 chance this salesman is involved.
Given daily sales counts of 1 2 2 4 1 4 3 2 4 1 3 3 2 4 3 3 2 3 3, do you think the salesman is lying?

Binomial Example

Example

Data: 1 2 2 4 1 4 3 2 4 1 3 3 2 4 3 3 2 3 3

- $\mathcal{M} = 1$ - From $P_1(x|p)$ a binomial distribution Binomial(4). Prior on p is uniform.
- $\mathcal{M} = 2$ - From $P_2(x)$ a uniform distribution Uniform(0,...,4).
- Discuss what you would do?
- $P(\mathcal{M} = 1) = 0.8$.

Binomial Example

Example

Data: 1 2 2 4 1 4 3 2 4 1 3 3 2 4 3 3 2 3 3

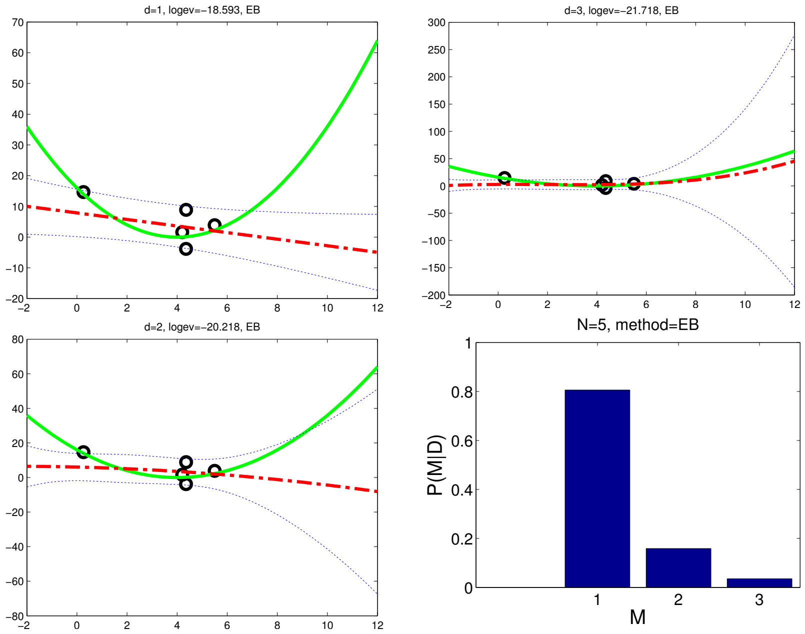
- $\mathcal{M} = 1$ - From $P_1(x|p)$ a binomial distribution Binomial(4). Prior on p is uniform.
- $\mathcal{M} = 2$ - From $P_2(x)$ a uniform distribution Uniform(0,. . . ,4).
- $P(\mathcal{M} = 1) = 0.8$.

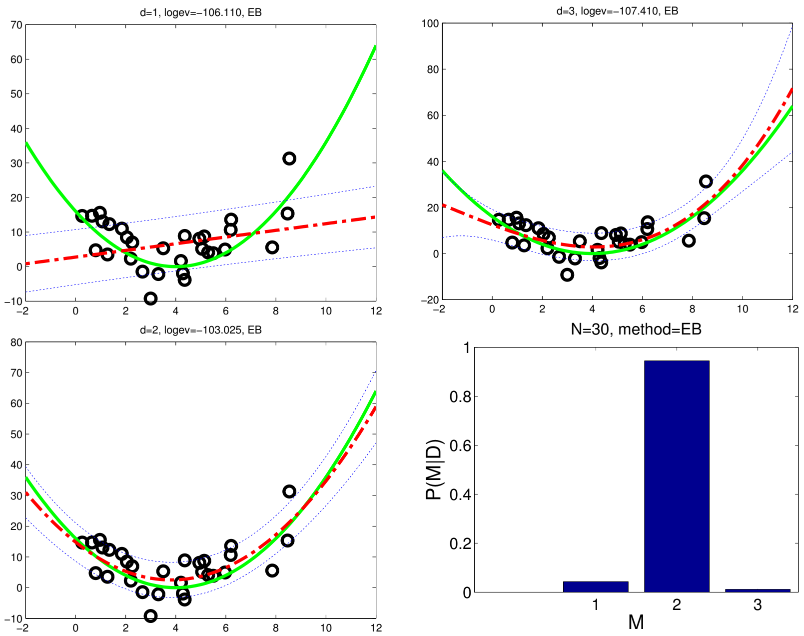
$$P(\mathcal{D}|\mathcal{M} = 1) = \int dp\ P_1(\mathcal{D}|p)P(p)\ ,\ P(\mathcal{D}|\mathcal{M} = 2) = P_2(\mathcal{D})$$

$$P(\mathcal{M}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{M})P(\mathcal{M})}{P(\mathcal{D}|\mathcal{M} = 1)P(\mathcal{M} = 1) + P(\mathcal{D}|\mathcal{M} = 2)P(\mathcal{M} = 2)}$$

- Left as an exercise! (see tutorial)

Linear Regression Example





Summary

- Training and test error, overfitting
- Validation set, cross validation
- Bayesian Model Comparison