ST451 - Lent term
Bayesian Machine Learning

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Bayesian Inference Concepts - Linear Regression

Summary of last lecture

- Linear regression: $y \sim \mathrm{N}(X\beta, \sigma^2)$.
- MLE - Least Squares estimator: $\hat{\beta} = (X^T X)^{-1} X^T y$. Minimises
$$\sum_{i=1}^{n} (y_i - \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p)^2,$$
- Ridge regression estimator $\hat{\beta}^r = (X^T X + \lambda^2 I)^{-1} X^T y$ corrects for overfit by minimisong
$$\sum_{i=1}^{n} (y_i - \beta_0 + \beta_1 x_i + \cdots + \beta_p x_p)^2 + \lambda \sum_{i=1}^{M} \beta_i^2.$$
- Same as Bayesian estimator obtained by assigning $N(0, \sigma^2 gI)$ as prior for β - Bayesian linear regression

Outline

Outline

Normal with unknown mean vs Linear Regression

Null model: Assume $y = (y_1, \ldots, y_n)$ (y_i independent) from $\mathrm{N}(\theta, \sigma^2)$ with σ^2 known. Assign $\mathrm{N}(\mu_0, \sigma^2\tau_0^2)$ as prior for θ.
The posterior $\pi(\theta|y, \sigma^2)$ is then $\mathrm{N}(\mu_n, \sigma^2\tau_n^2)$ where

$$\mu_n = \frac{\frac{1}{n}\mu_0 + \tau^2\bar{y}}{\tau^2 + \frac{1}{n}}, \quad \tau_n^2 = \frac{1}{\frac{1}{\tau^2}+n}$$

Linear Regression model: Assume y is $\mathrm{N}(X\beta, \sigma^2 I_n)$. Assign $\mathrm{N}(\mu_0, \sigma^2\Omega_0)$ as prior for β.
The posterior $\pi(\beta|y, X, \sigma^2)$ is then $\mathrm{N}(\mu_n, \sigma^2\Omega_n^2)$ where

$$\mu_n = (X^TX + \Omega_0^{-1})^{-1}(\Omega_0^{-1}\mu_0 + X^Ty), \quad \Omega_n = (X^TX + \Omega_0^{-1})^{-1}$$

What if σ^2 is unknown?

Bayesian inference for multiparameter models

We may have more than one parameters, say $\theta = (\theta_1, \theta_2)$. As before assign a prior $\pi(\theta_1, \theta_2)$ and obtain the posterior

$$\pi(\theta_1, \theta_2|y) = \frac{f(y|\theta_1, \theta_2)\pi(\theta_1, \theta_2)}{\int\int f(y|\theta_1, \theta_2)\pi(\theta_1, \theta_2)d\theta_1 d\theta_2}$$

If interest mainly lies in θ_1, the marginal posterior of θ_1 may be used by averaging over θ_2

$$\pi(\theta_1|y) = \int \pi(\theta_1, \theta_2|y)d\theta_2$$

Example 1: Normal with both μ and σ^2 unknown

Let $y = (y_1, \ldots, y_n)$ independent rv's from the N(θ, σ^2)

Likelihood: The likelihood is (s_y^2 denotes the sample variance)

$$f(y|\theta, \sigma^2) \propto (\sigma^2)^{-n/2} \exp\left(-\frac{(n-1)s_y^2 + n(\bar{y} - \theta)^2}{2\sigma_y^2}\right)$$

Prior: Assume an improper prior $\pi(\theta, \sigma^2) \propto (\sigma^2)^{-1}$

Example 1: Posterior

Posterior: factorised as $\pi(\theta, \sigma^2|y) = \pi(\sigma^2|y)\pi(\theta|y, \sigma^2)$

$$\pi(\theta, \sigma^2|y) \propto (\sigma^2)^{-n/2-1} \exp\left(-\frac{(n-1)s_y^2 + n(\bar{y}-\theta)^2}{2\sigma^2}\right)$$

$$= (\sigma^2)^{-n/2-1} \exp\left(-\frac{(n-1)s_y^2}{2\sigma^2}\right) \exp\left(-\frac{(\bar{y}-\theta)^2}{2\frac{\sigma^2}{n}}\right)$$

$$\propto (\sigma^2)^{-n/2-1} \exp\left(-\frac{(n-1)s_y^2}{2\sigma^2}\right) \frac{(\frac{\sigma^2}{n})^{1/2}}{(\frac{\sigma^2}{n})^{1/2}} \exp\left(-\frac{(\theta-\bar{y})^2}{2\frac{\sigma^2}{n}}\right)$$

$$= (\sigma^2)^{-(n-1)/2-1} \exp\left(-\frac{\frac{(n-1)s_y^2}{2}}{\sigma^2}\right) \mathrm{N}\left(\bar{y}, \frac{\sigma^2}{n}\right)$$

$$= \mathrm{IGamma}\left(\frac{n-1}{2}, \frac{(n-1)s_y^2}{2}\right) \times \mathrm{N}\left(\bar{y}, \frac{\sigma^2}{n}\right)$$

Note: the above IGamma(), N() refer to the corresponding pdfs

Example 1: Proper priors

Aiming for a proper prior we can set as in the previous slide

$$\pi(\theta, \sigma^2) = \pi(\sigma^2)\pi(\theta|\sigma^2) = \text{IGamma}(\alpha_0, \beta_0) \times \text{N}(\mu_0, \sigma^2\tau_0^2)$$

Similar calculations the yield that $\pi(\theta, \sigma^2|y)$ can be factorised as

$$\pi(\theta, \sigma^2|y) = \pi(\sigma^2|y)\pi(\theta|\sigma^2, y) = \text{IGamma}(\alpha_n, \beta_n) \times \text{N}(\mu_n, \sigma^2\tau_n^2)$$

where

$$\mu_n = \frac{\frac{1}{n}\mu_0 + \tau_0^2\bar{y}}{\tau_0^2 + \frac{1}{n}}, \qquad \tau_n^2 = \frac{1}{\frac{1}{\tau_0^2} + n},$$

$$\alpha_n = \alpha_0 + n/2, \quad \beta_n = \beta_0 + \frac{n-1}{2}s_y^2 + \frac{\frac{1}{\tau^2}n(\bar{y}-\mu_0)^2}{2(1/\tau_0^2+n)}$$

Bayesian Linear Regression model with unknown σ^2

Assume y is N($X\beta, \sigma^2 I_n$). Assign N($\mu_0, \sigma^2\Omega_0$) as prior for β (given σ^2) and the IGamma(α_0,β_0) for σ^2.

The posterior for $\pi(\beta, \sigma^2|y, X)$ is then the product of the IGamma(α_n, β_n) and the N($\mu_n, \sigma^2\Omega_n^2$) where

$$\begin{aligned}
\mu_n &= (X^T X + \Omega_0^{-1})^{-1}(\Omega_0^{-1}\mu_0 + X^T y) \\
\Omega_n &= (X^T X + \Omega_0^{-1})^{-1}, \\
\alpha_n &= \alpha_0 + \frac{n}{2}, \\
\beta_n &= \beta_0 + \frac{1}{2}(y^T y + \mu_0^T \Omega_0^{-1}\mu_0 + \mu_n^T \Omega_n^{-1}\mu_n).
\end{aligned}$$

Example 1: Marginal posterior of μ

For the improper prior case, The joint posterior is

$$\pi(\theta, \sigma^2|y) \propto (\sigma^2)^{-n/2-1} \exp\left(-\frac{(n-1)s_y^2 + n(\bar{y}-\theta)^2}{2\sigma^2}\right)$$

Integrating σ^2 out yield the marginal posterior of θ to be the *t* distribution with $n-1$ degrees of freedom, location $\bar{y}$ and scale $s_y/\sqrt{n}$

Bayesian Linear Regression model with unknown σ^2

Assume y is N($X\beta, \sigma^2 I_n$). Assign N($\mu_0, \sigma^2\Omega_0$) as prior for β (given σ^2) and the IGamma(α_0,β_0).

The posterior for $\pi(\beta, \sigma^2|y, X)$ is then the product of the IGamma(α_n, β_n) and the N($\mu_n, \sigma^2\Omega_n^2$) where

$$\begin{aligned}
\mu_n &= (X^T X + \Omega_0^{-1})^{-1}(\Omega_0^{-1}\mu_0 + X^T y) \\
\Omega_n &= (X^T X + \Omega_0^{-1})^{-1}, \\
\alpha_n &= \alpha_0 + \frac{n}{2}, \\
\beta_n &= \beta_0 + \frac{1}{2}(y^T y + \mu_0^T \Omega_0^{-1}\mu_0 + \mu_n^T \Omega_n^{-1}\mu_n).
\end{aligned}$$

The marginal posterior for β, $\pi(\beta|y, X)$ is the multivariate t distribution with $2\alpha_n$ degrees of freedom, location μ_n and scale $\frac{\beta_n}{\alpha_n}\Omega_n$

Marginal Posterior of β and Predictive distribution

To obtain credible intervals for β we could use the *t* distribution. But we would use Monte Carlo instead as this will cover more general models. e.g. logistic regression.

So we will sample N Monte Carlo samples from $\pi(\beta|y)$ and use them for Monte Carlo inference (credible intervals, density plots etc)

Monte Carlo Samples can be drawn by

1. Generating samples σ_i^2 from IGamma(α_n, β_n), $i = 1, \ldots, N$,
2. Draw β_i sample based on each σ_i^2 from N$(\mu_n, \sigma^2\Omega_n^2)$,

For the predictive distribution for a new observation $y*$ based on covariates X_* we can use the additional step of drawing y_{*i} from $N(X_*\beta_i, \sigma_i^2)$ for each β_i, σ_i^2.

Outline

Example: Automobile Bodily Injuries Claim data

The data are automobile injury claims from the Insurance Research Council (IRC) collected in 2002.

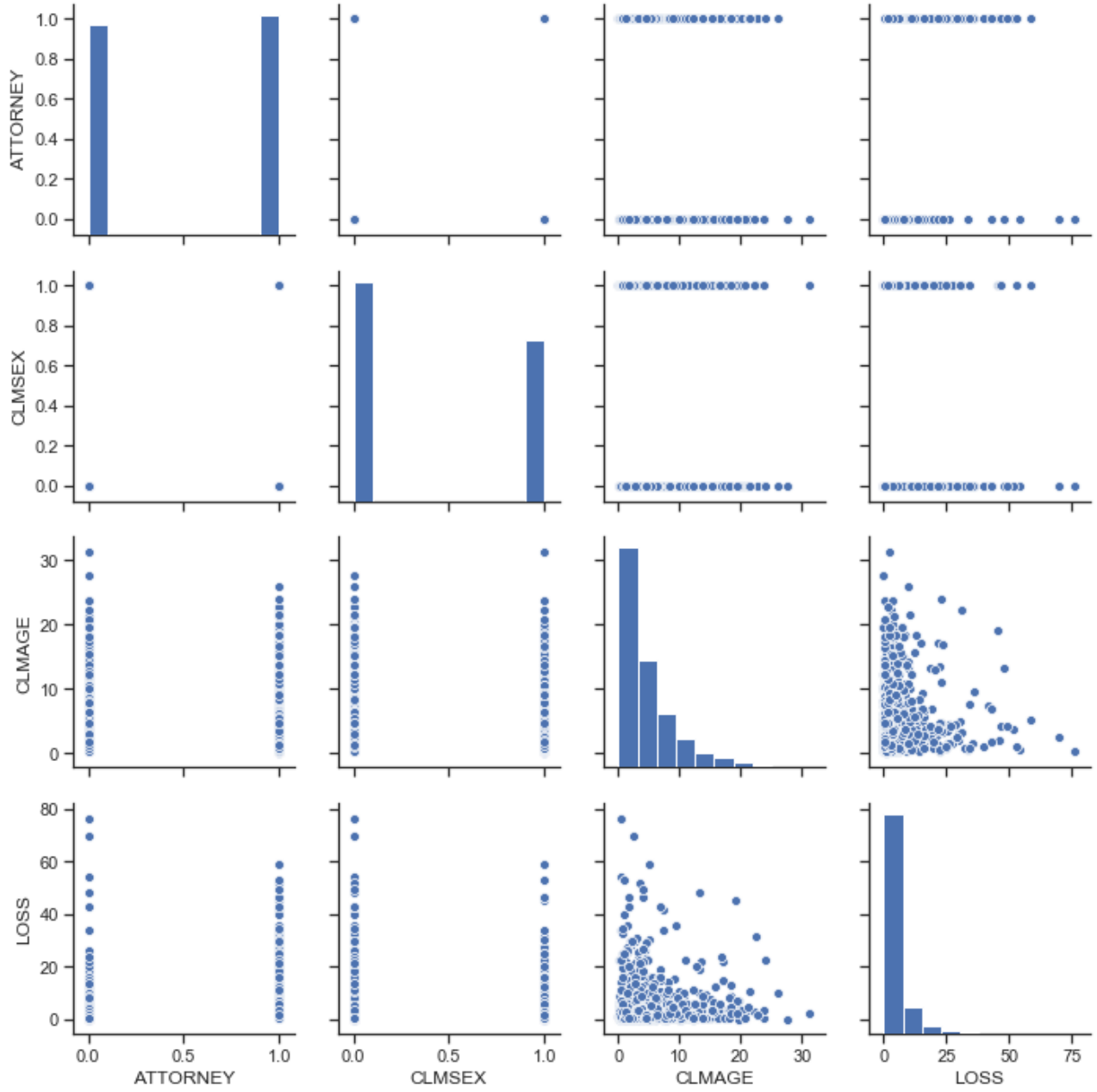
They contain information on the gender of the claimant, attorney involvement, years of driving experience and the economic loss (in thousands $).

Is the information on the claimant's gender an important predictor? As of now insurers are not allowed to use gender information.

The hypothesis testing / model selection problem can be formulated as the Bayes factor between the model including all the variables and the model without gender. Or else if we fit the model with all variables

$$H_0 : \beta_{gender} = 0 \quad \text{vs} \quad H_1 : \beta_{gender} \neq 0$$

Example: Automobile Bodily Injuries Claim data



Bayesian Hypothesis Testing / Model Choice

Hypotheses: Let $H_0 : \theta \in \Theta_0$ and $H_1 : \theta \in \Theta_1$.

Define the Bayes factor in favour of H_1 as $B_{10}(x) = f(x|H_1)/f(x|H_0)$.
The Bayes test rule is Choose H_1 if $B_{10}(x) > 1$.

Notes

- No control of type I error probability.
- Simple outcome, reference to both hypotheses, choice of H_0 vs H_1 doesn't matter, easily extended to more hypotheses.

The Bayes factor can be computed from either of the expressions below

$$B_{10}(x) = \frac{\int_{\Theta_1} f(x|\theta, H_1)\pi(\theta|H_1)d\theta}{\int_{\Theta_0} f(x|\theta, H_0)\pi(\theta|H_0)d\theta} = \frac{P(H_1|x)/P(H_0|x)}{P(H_1)/P(H_0)}$$

Bayes factor - interpretation

In terms of interpretation the following guidelines are available

$1 < B_{10}(x) \leq 3$	evidence against H_0 is **poor**
$3 < B_{10}(x) \leq 20$	evidence against H_0 is **substantial**
$20 < B_{10}(x) \leq 150$	evidence against H_0 is **strong**
$B_{10}(x) > 150$	evidence against H_0 is **decisive**

Bayesian Occam's razor

Bayesian Occam's razor: Models with more parameters (more complex models) will not necessarily have higher marginal likelihood.

Conservation of probability mass: More complex models will handle more complex datasets adequately. But the probabilities over all these datasets will have to sum to one.

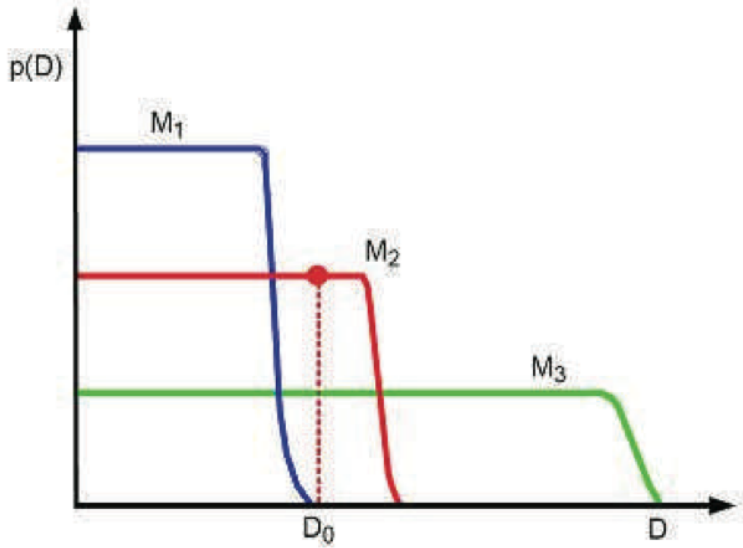


Figure 5.6 A schematic illustration of the Bayesian Occam's razor. The broad (green) curve corresponds to a complex model, the narrow (blue) curve to a simple model, and the middle (red) curve is just right. Based on Figure 3.13 of (Bishop 2006a). See also (Murray and Ghahramani 2005, Figure 2) for a similar plot produced on real data.

Jeffreys-Lindley-(Bartlett) paradox - example 1

Real data example: A person claimed to possess extrasensory capacities (ESP) and can alter the outcome of a machine that output $0, 1$ with probability $\theta = 0.5$ (H_0). H_1 is $\theta \neq 0.5$.

In 104.490.000 trials, there were 52.263.471 ones.

Jeffreys-Lindley-(Bartlett) paradox - example 1

Maybe not a paradox. Frequentist testing ask the question is $\theta = 0.5$?

Bayesian testing compares a model with $\theta = 0.5$ and a model with θ drawn uniformly from $(0, 1)$ as to how they explain the data.

Jeffreys-Lindley-(Bartlett) paradox - example 2

Let $y = (y_1, \ldots, y_n)$ iid from the N(θ,1) distribution, and consider testing $H_0 : \theta = 0$ vs $H_1 : \theta \neq 0$.

The Bayes factor is

$$B_{01} = \frac{\exp\{-n(\bar{y}_n)^2/2\}}{\int_{-\infty}^{+\infty} \exp\{-n(\bar{y}_n - \theta)^2/2\}\pi(\theta)\,\mathrm{d}\theta}$$

Assume the improper Jeffreys prior $p(\theta) = c$. Then

$$B_{01} = \frac{\exp\{-n(\bar{y}_n)^2/2\}}{c\int_{-\infty}^{+\infty} \exp\{-n(\bar{y}_n - \theta)^2/2\}\,\mathrm{d}\theta} = \frac{\exp\{-n(\bar{y}_n)^2/2\}}{c\sqrt{2\pi/n}}$$

The decision depends on the arbitrary constant c! Should use proper priors.

Jeffreys-Lindley-(Bartlett) paradox - example 2 (cont'd)

Consider the low informative prior $\mathrm{N}(0, \tau^2)$ with some big τ^2. The Bayes factor is

$$B_{01} = \frac{\exp\{-n(\bar{y}_n)^2/2\}}{\int_{-\infty}^{+\infty} \exp\{-n(\bar{y}_n - \theta)^2/2\}(2\pi\tau^2)^{-1/2} \exp(-\theta^2/2\tau^2)\, \mathrm{d}\theta}$$

As $\tau \to \infty$, $B_{01} \to \infty$ regardless of $\bar{y}_n$ (except if $\bar{y}_n = 0$). So we for a near-infinite value of τ^2 we will always choose H_0.

It is therefore clear that more thought should be put on the choice of $\pi(\theta)$ when it come to testing.

If we don't have information we still need to put some information but not too much.

Unit information priors

In the previous example the unit information prior is the $N(\mu_0, 1)$, i.e. putting the same prior variance as the variance of each data point.

The posterior is $\mathrm{N}(\mu_n, \tau_n^2)$ with

$$\mu_n = \frac{1}{n+1}(\mu_0 + n\bar{y}), \quad \tau_n^2 = \frac{1}{n+1}$$

This prior is like adding one more observation equal to μ_0. In fact σ^2 corresponds to Fisher information from one data point.

Cheat (add information), but as little as possible.

Unit information prior for Linear Regression

In the linear regression case remember from the derivation of MLE that

$$\frac{\partial}{\partial \beta} \log f(y|X, \widehat{\beta}, \sigma^2) = \frac{1}{\sigma^2} \left(\sum_{i=1}^{n} X_i^T Y_i - \sum_{i=1}^{n} X_i^T X_i \widehat{\beta} \right),$$

Hence the Fisher information for β based on n observations is

$$I(\beta) = -E\left[-\frac{1}{\sigma^2} X^T X \right] = \frac{X^T X}{\sigma^2}$$

Unit information takes the average over n observations so the variance is set to $n\sigma^2 (X^T X)^{-1}$.

This implies setting $\Omega_0 = n(X^T X)^{-1}$, so $(X^T X)^{-1}$ instead of I_p and with $g = n$.

Bayesian Model Selection

To compare models we will need to compute the marginal likelihood or evidence for each model.

We can then use the model with the highest marginal likelihood. The use of unit information prior is the default option to guard against the Jeffreys-Lindley paradox.

Computing the marginal likelihood is generally a very difficult task but here we can use the following trick. We can write

$$\pi(\beta, \sigma^2|y, X) = \frac{\pi(y|\beta, \sigma^2, X)\pi(\beta, \sigma^2)}{\pi(y|X)}, \text{ or else}$$

$$\pi(y|X) = \frac{\pi(y|\beta, \sigma^2, X)\pi(\beta, \sigma^2)}{\pi(\beta, \sigma^2|y, X)}, \text{ for all } \beta, \sigma^2.$$

The expression above contains known Normal and Inverse Gamma pdfs so we can just evaluate for -say- the posterior mean of β, σ^2.

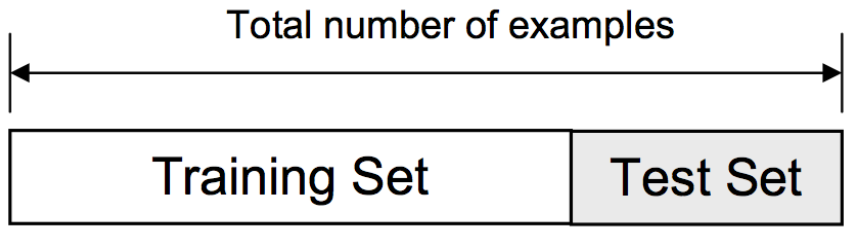
Outline

Training error versus Test error

- In machine learning the choice between models or priors (tuning parameters) is made on the basis of their out of sample performance.
- Models are estimated in part(s) of the data, the training set. The training error can be found by checking predictions of each model on the the training set data.
- The test set consists of data not used in the training set. The test error is the obtained by checking the predictions of each model, estimated (trained) on the training data.
- Training error often is quite different from the test error; the former can dramatically underestimate the latter.

Hold out method

The method described in the previous slide is also known as holdout method.



The holdout method has two basic drawbacks:

- In problems where we have a sparse dataset we may not be able to afford the luxury of setting aside a portion of the dataset for testing
- Since it is a single train-and-test experiment, the holdout estimate of error rate will be misleading if we happen to get an unfortunate split

Cross Validation

The drawback above can be overcome by using resampling methods at the expense of a higher computational cost.

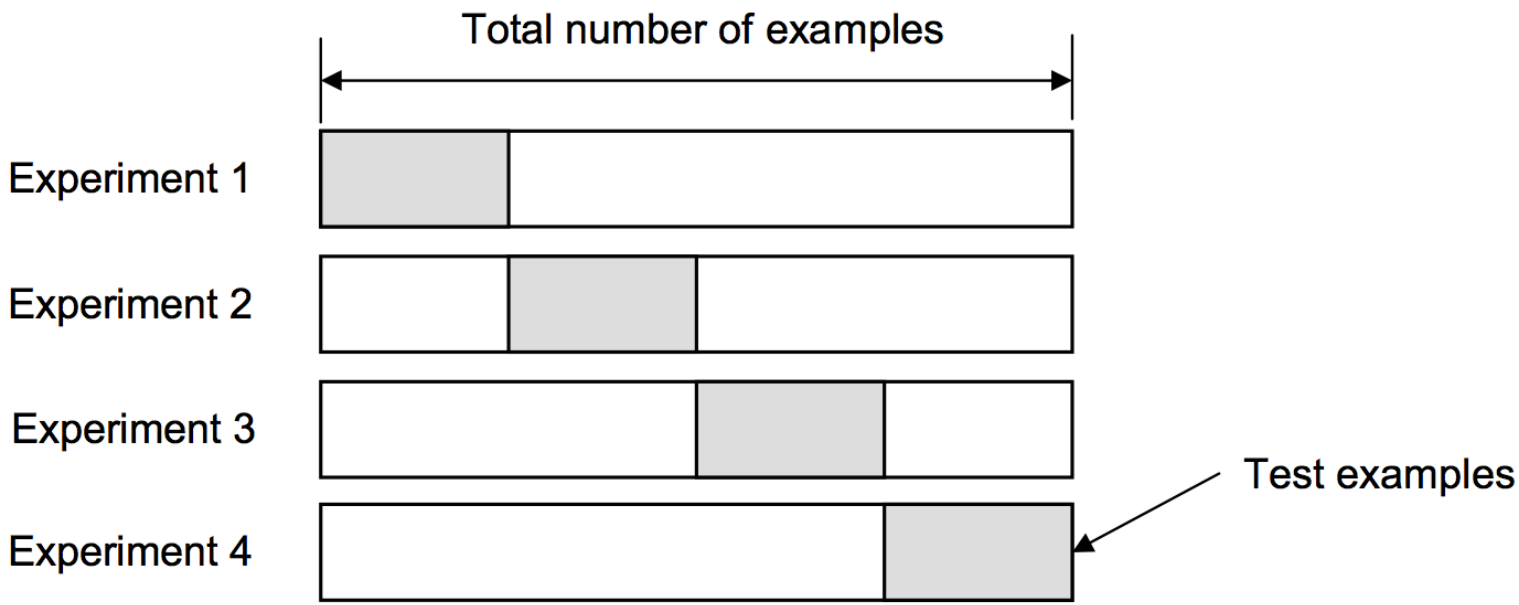
One of them is cross-validation. The following are the most frequently used cross-validation techniques:

- Random Subsampling
- K-Fold Cross-Validation
- Leave-one-out Cross-Validation

In all of the above schemes several train-test splits are constructed and the test error is averaged over them.

K-Fold Cross Validation

- For each of K experiments, use $K - 1$ folds for training and a different fold for testing.
- K-Fold Cross validation is similar to Random Subsampling. The advantage is that all the examples in the dataset are eventually used for both training and testing



How many folds are needed? (cont'd)

In practice, the choice of the number of folds depends on the size of the dataset

- For large datasets, even 3-Fold Cross Validation will be quite accurate
- For very sparse datasets, we may have to use leave-one-out in order to train on as many examples as possible

Test error and model selection

- If model selection and test error estimates are to be computed simultaneously, the data needs to be divided into three disjoint sets [Ripley, 1996]:
  1. Training set: to train different versions of each model.
  2. Validation set: to tune the parameters of each model and compare.
  3. Test set: For estimating the test error of the best model.

- Test and validation sets are separated because the error rate estimate of the final model on validation data will be biased downwards.

- After assessing the final model on the test set, you must not tune the model any further.

Today's lecture - Reading

Murphy: 5.3 and 7.6

Bishop: 2.3.6, 3.3.1, 3.3.2, 3.4, 3.5.1 and 3.5.2