ECON484 Machine Learning

1. Concepts of Machine Learning (2/2)

Lecturer:

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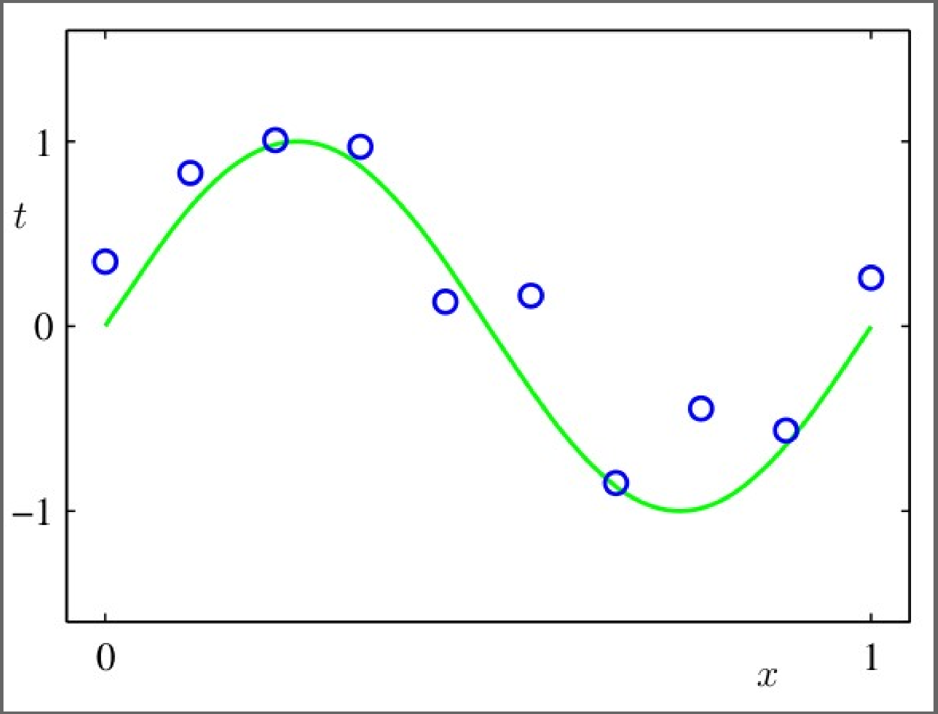
An Applied Example

- We will look at the basic problem of polynomial curve fitting (adapted from Bishop 2006).
  - This will involve optimizing the parameters (polynomial coefficients) ad be classified as an estimation problem.
  -

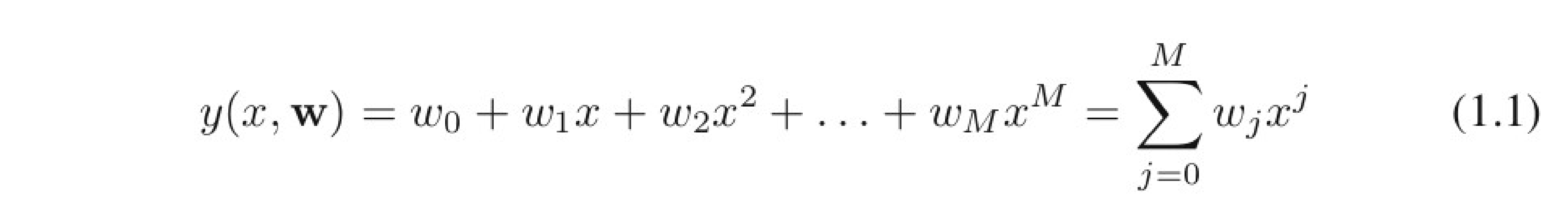
An Applied Example

- Our actual function is a sine wave $t=\sin(2\pi x)$.
  - We are given a training set $X=(x_1, x_2, \ldots, x_N)^T$
  - The data set has generated data and some (Gaussian) noise.



An Applied Example

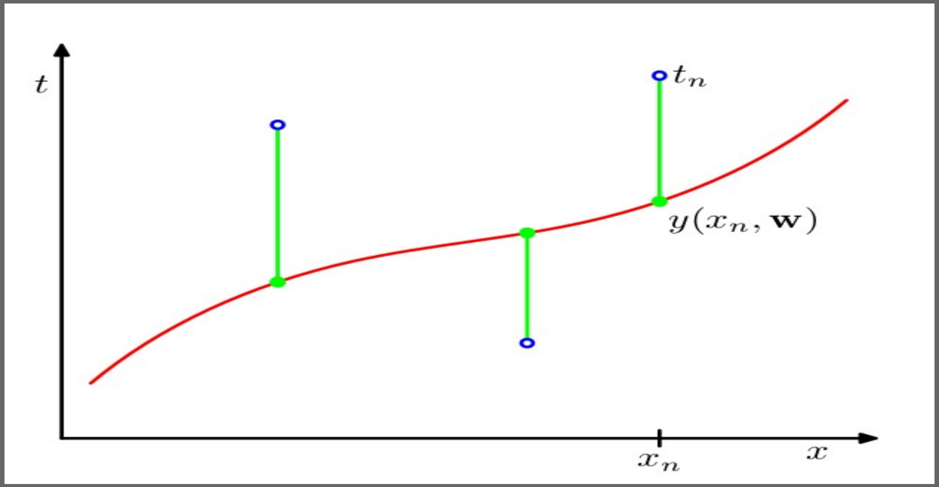
- We should have a model and the model parameters.
  - w=(w_0, w_1,w_2,...w_M) are the model parameters where M is the dimension of the polynomial.



$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j \qquad (1.1)$$

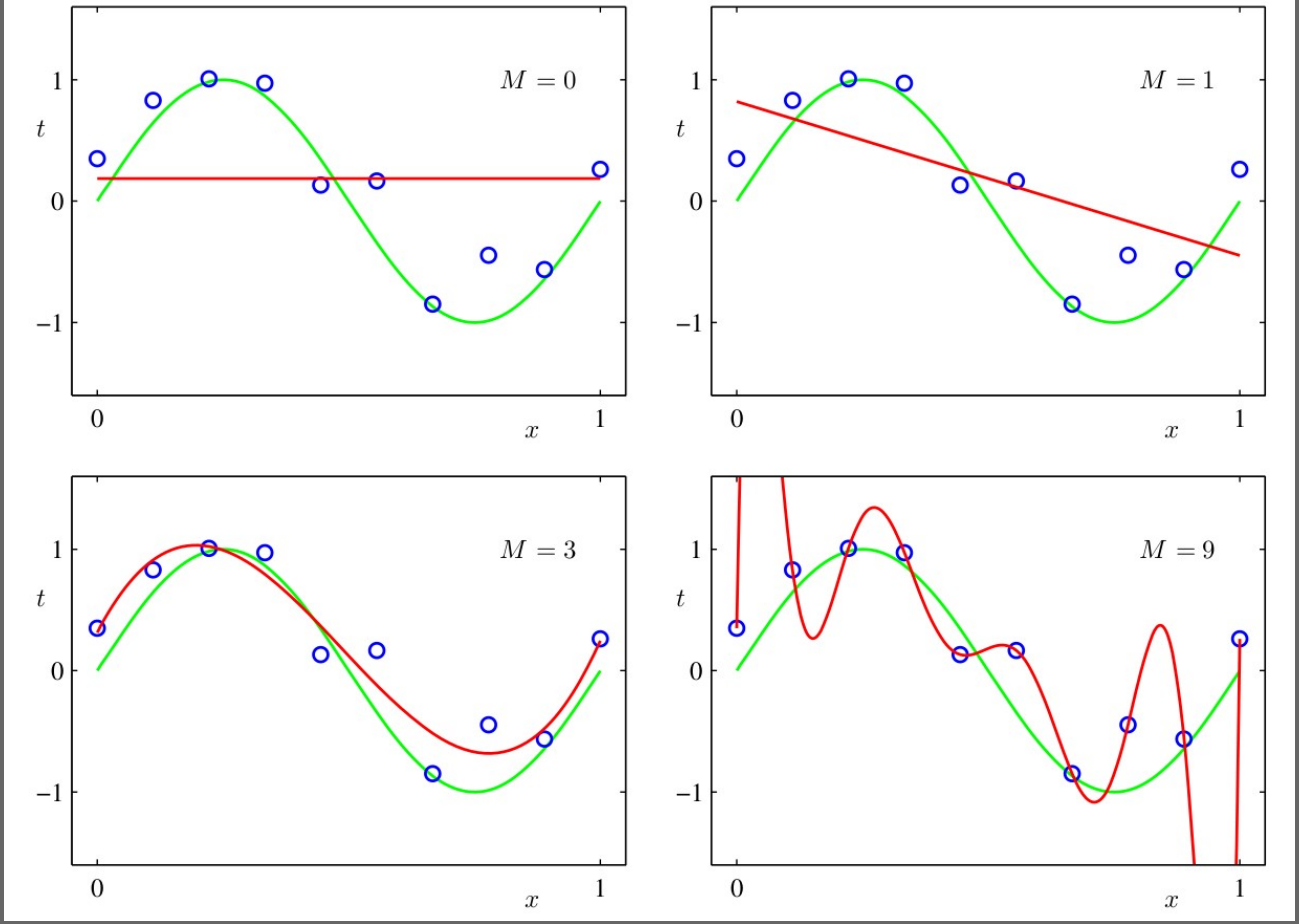
An Applied Example

- Our parameter estimation problem is now expressed as “estimate **w** (as vector) to minimize”.
  - Error is defined as E(w) which is calculated using estimated y_N and actual t_N in the training set.



$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 \qquad (1.2)$$

An Applied Example

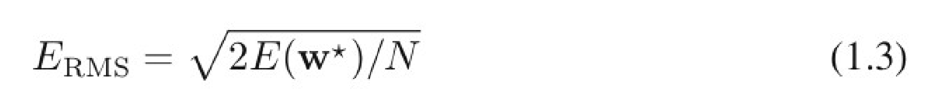


An Applied Example

- M=3 has more error in the training data set than M=9, however it will give a better overall fit for the curve.
    - This is why actual performance should be measured with practical application.
    - The problem with M=9 is what we call **over-fitting**.

An Applied Example

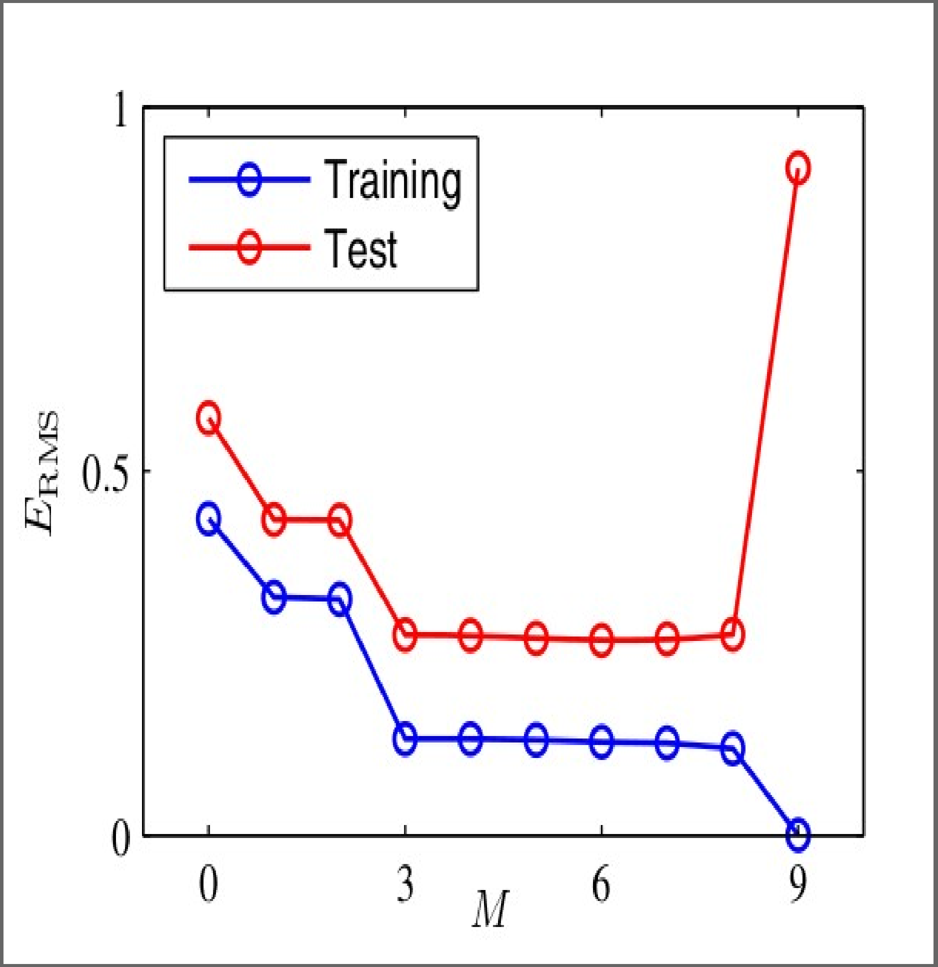
- To measure performance, we generate a new test data set (again by adding noise) of size 100.
  - Then we define the error measure as E_{RMS}.
  - Let’s calculate E_{RMS}



$$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N} \tag{1.3}$$

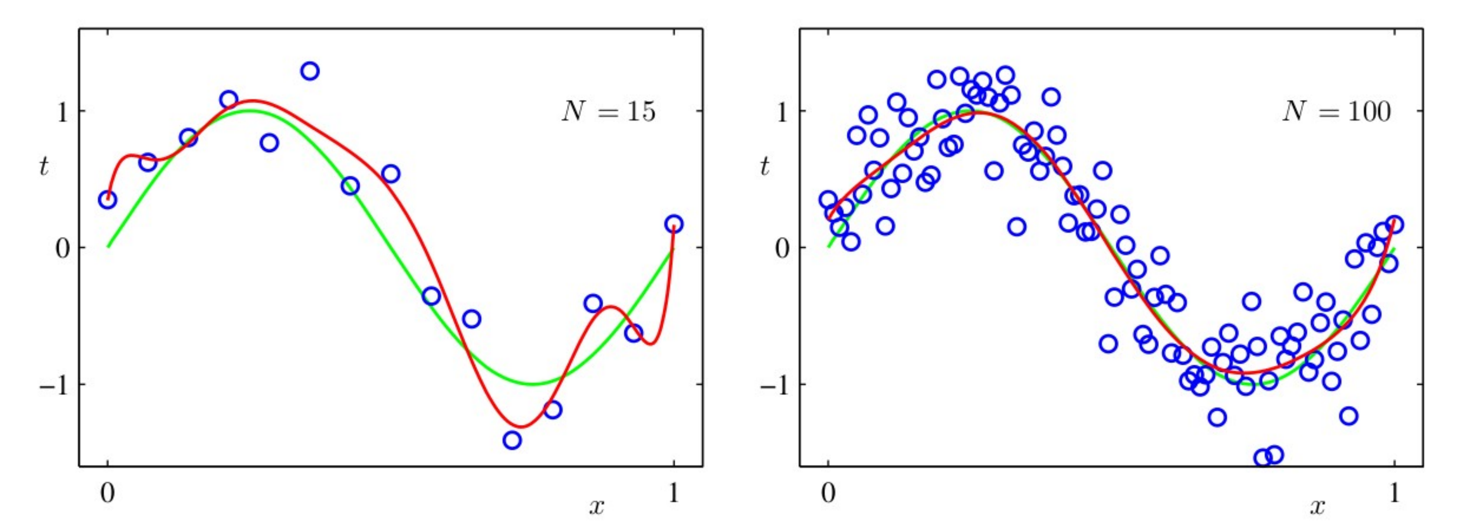
An Applied Example

- What we see
  - In the overtrained model, E_{RMS} increases wildly with test data set.
  - From M=3 to M=8 the error looks minimal.
  - So we keep the simplest form, M=3.



An Applied Example

- A way to reduce the error with M=9 model would be to train with a larger training data set.



An Applied Example

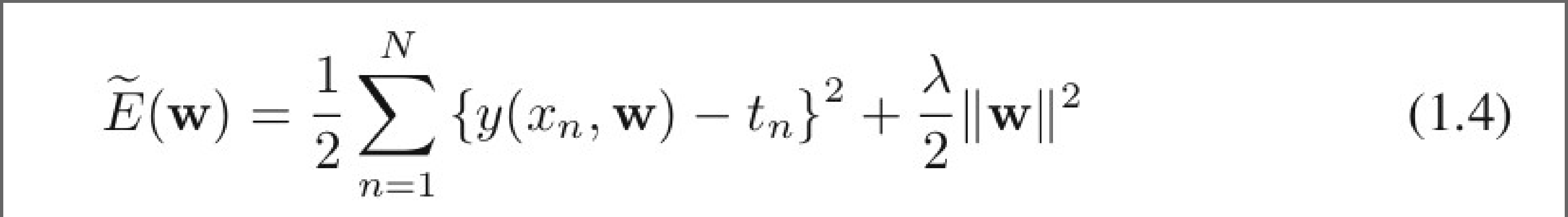
- It seems that having a larger training data set solves some problems.
  - But it is not practical to assume we have a larger training data set in all practical settings.
  - One approach is to retrain our data models frequently.
  - Another approach is to employ different models.
- Model complexity should reflect the complexity of the real world.

An Applied Example

- In the example case, the reason for the large fluctuation of estimated values is the very large coefficients in the model we obtain after training.
    - The better models include smaller coefficients.
    - So why not penalize very large coefficients in the model?

An Applied Example

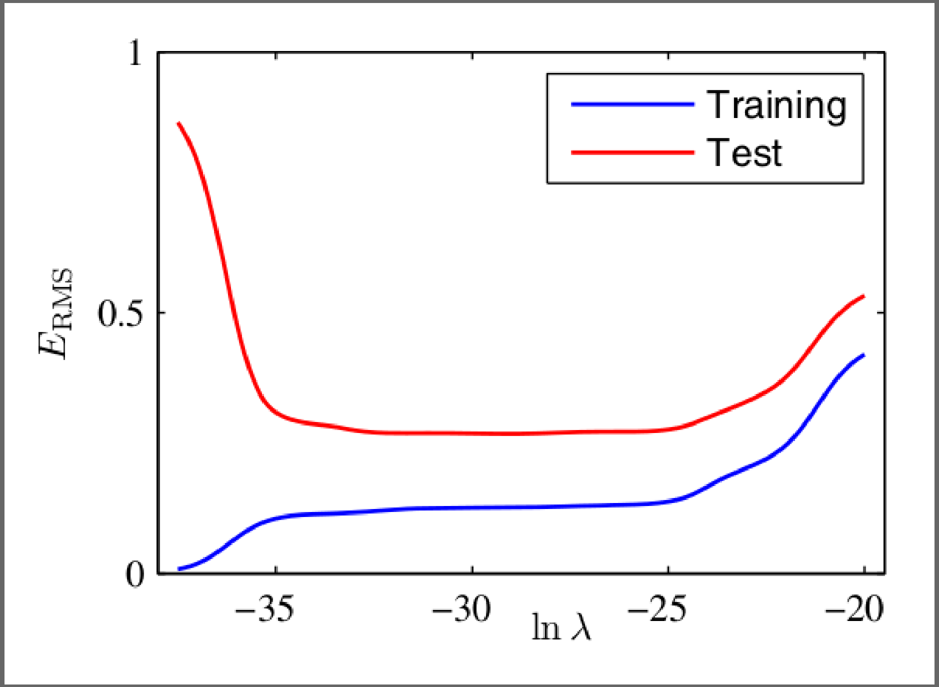
- We penalize very large coefficients through a modified error definition.
  - This modification type is called a **shrinkage** (or **weight decay**), and this particular one is called a **ridge regression**.



$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2 \qquad (1.4)$$

An Applied Example

- Our selection of model modification has added a new parameter to optimize
  - **Lambda** which symbolized how important the shrinkage is.
  - We should also select this parameter.

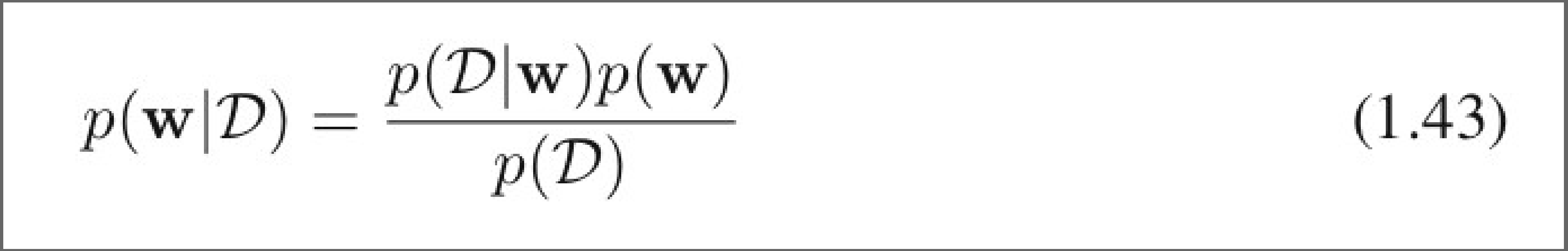


An Applied Example

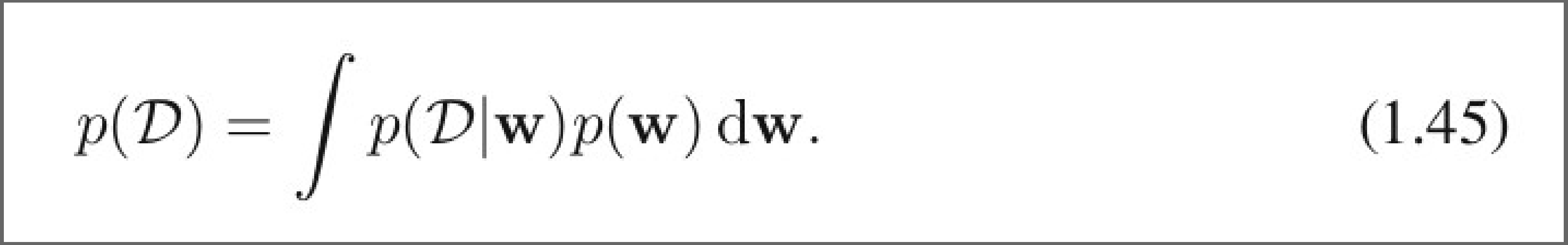
- Another approach to the same estimation problem would be Bayesian.
  - Let our training data $D=(t_1, t_2, \ldots, t_N)$ represent a number of observations.
  - Let us assume our parameter set **w** is now probabilistic with a probability distribution **p(w)**.
  - We try define all quantities as a function of **w**.

An Applied Example

- With p(D|w) as the likelihood function:



$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})} \qquad (1.43)$$



$$p(\mathcal{D}) = \int p(\mathcal{D}|\mathbf{w})p(\mathbf{w})\,\mathrm{d}\mathbf{w}. \qquad (1.45)$$

An Applied Example

- With the frequentist school of thought, we usually use a maximum likelihood estimator, to maximize the likelihood function p(D|w).
  - The error is defined as the negative logarithm of likelihood function. As one increases the other should decrease.
  - However the fundamental difference is that we see **w** as a constant and discuss the variation of D given a **w**.

An Applied Example

- With the Bayesian school of thought, there is only the observations D, and we evaluate the uncertainty in w, after we observed D.
    - Therefore D is a constant, and there is a variation in w, which we discuss (and optimize).
- Also note that the likelihood function is not a probability distribution.
- The Bayesian approach requires a lot more computation than the frequentist approach, and is often infeasible to compute by hand.
    - But with computer resources at hand, it has become more popular.

An Applied Example

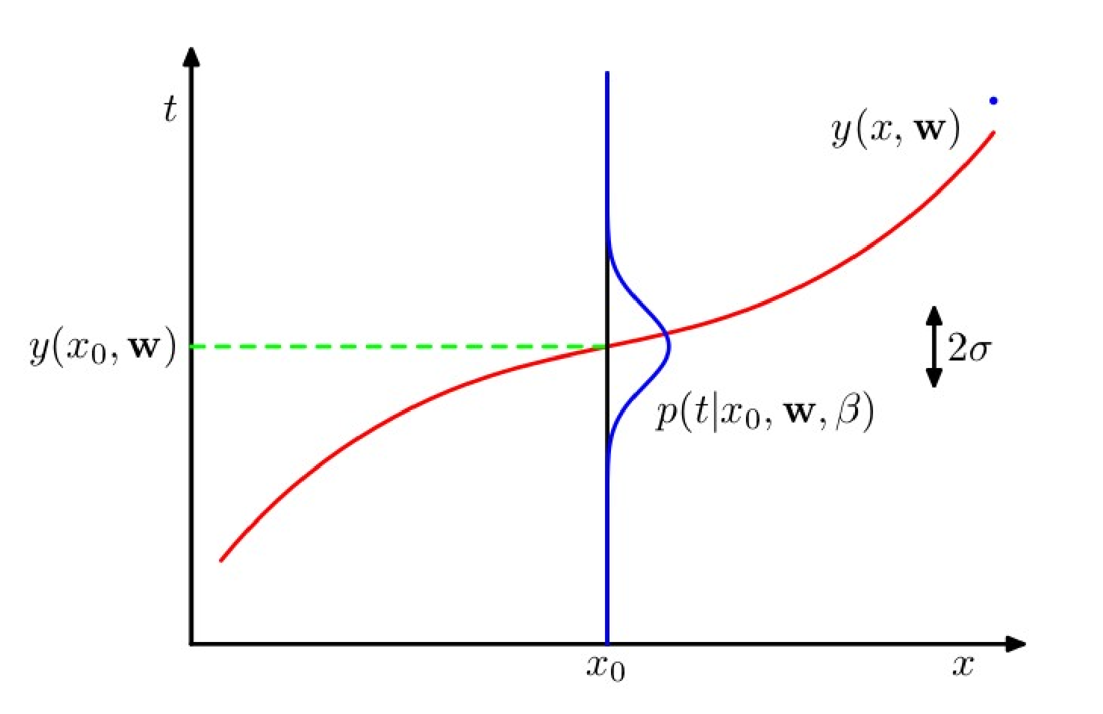
- So how to approach curve fitting from a Bayesian perspective?
  - We treat the observations $t=(t_1,t_2, .., t_N)^T$ as having some uncertainty with a selected probability density function (pdf). Our **model selection** is now based on our choice of PDF.
    - This is a **very big** issue. Frequentists often criticize Bayesian approach saying “selection of PDF after observation of training data is cheating”.
  - Let’s assume that the distribution of error is Gaussian (which we know to be true in this case).

An Applied Example

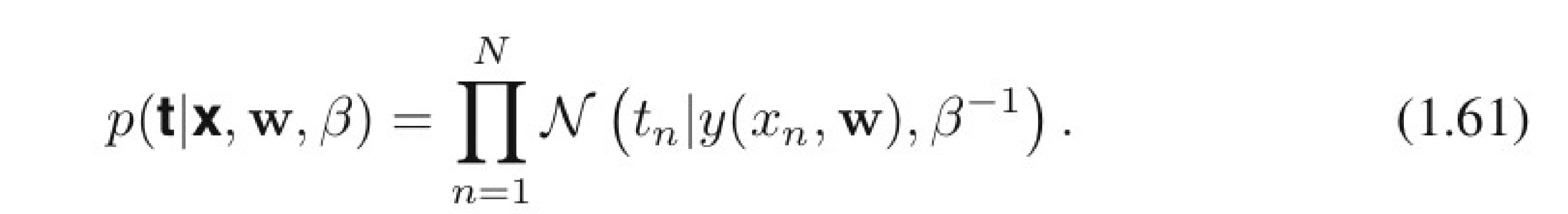
- With this model selection any observation t has now a conditional probability based on x with the parameters **w**, and beta.
  - We use the training data set and a **maximum likelihood estimator to find the parameter values**.
  - In order to minimize error, defined as negative logarithm of the maximum likelihood function, we will try to **maximize the logarithm of the maximum likelihood function**, with respect to beta.
  - Once we have the parameters, we can start making predictions.

An Applied Example

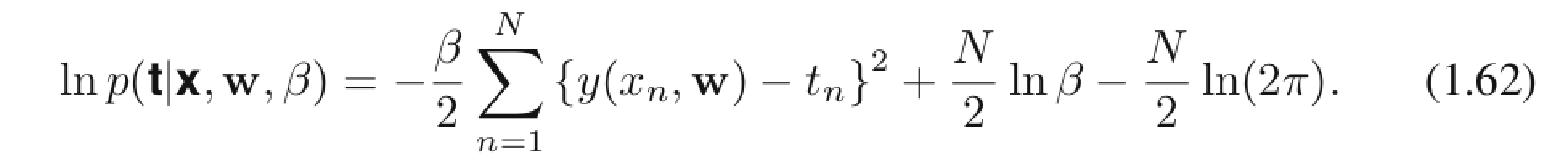
$$p(t|x, \mathbf{w}, \beta) = \mathcal{N}\left(t|y(x, \mathbf{w}), \beta^{-1}\right) \quad (1.60)$$



An Applied Example

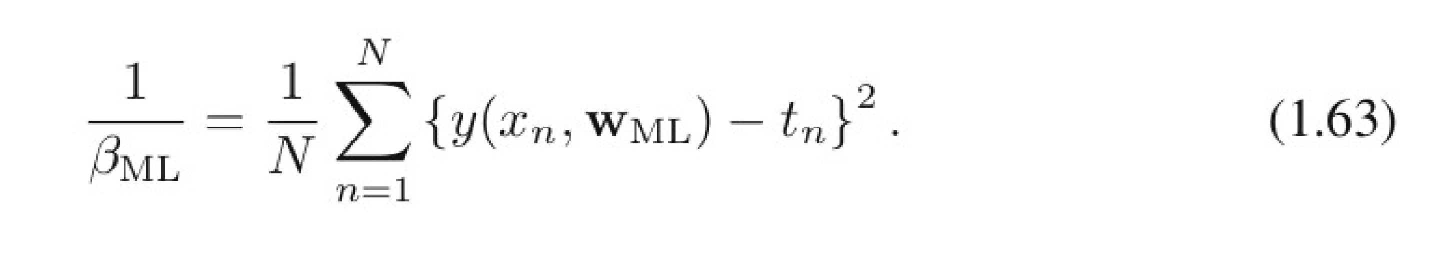


$$p(\mathsf{t}|\mathsf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n|y(x_n, \mathbf{w}), \beta^{-1}\right). \qquad (1.61)$$



$$\ln p(\mathsf{t}|\mathsf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi). \qquad (1.62)$$

An Applied Example



$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}_{\mathrm{ML}}) - t_n\}^2 . \qquad (1.63)$$

- Having determined w and beta, we can make predictions.
  - What we have is a predictive distribution p(t | x, w, beta) which gives **a probability distribution over t, not a point estimate.**
  - We could also assume w is probabilistic, and have **hyperparameters** on the distribution of w. For example **p(w|alpha)**.

An Applied Example

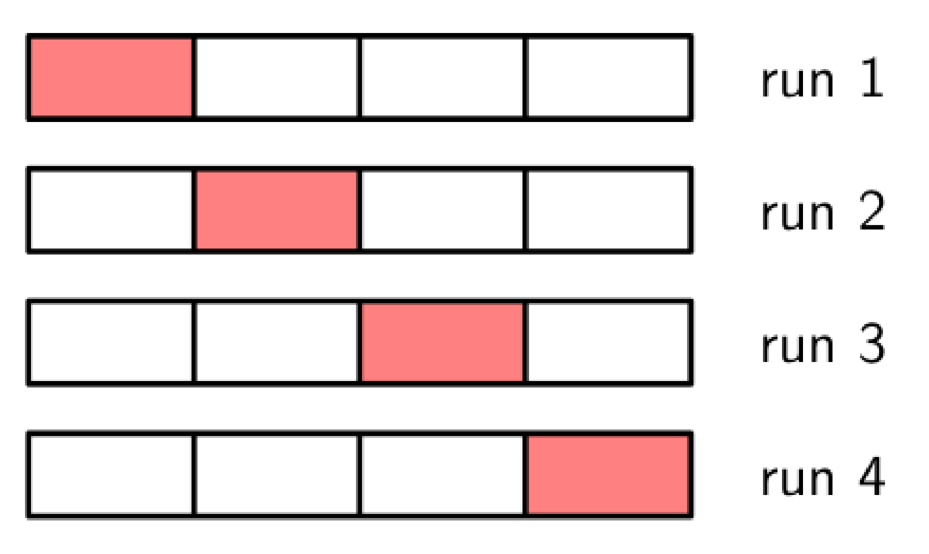
- When we assume w is probabilistic, we estimate the **most likely value of w given the observations D**.
  - This is equivalent to minimizing the error function to find w.
  - Note that in Bayesian approach we take integrals which is computationally expensive.
- In the maximum likelihood approach we have demonstrated the importance of overfitting, and having a large training data set.
- In the Bayesian approach we have demonstrated how complex it could become, and how much computation intensive our tasks can become.

How to work with a small training data set?

- This is an essential question.
  - When there is a large training data set, we select some for training and some for validation.
  - When there is a small training data set, we employ **cross-validation**.
    - In this approach, we have multiple runs, each time with a different part of the training set reserved for validation.
    - We develop descriptive statistics (ie. averages) from the performance of these runs and evaluate the performance based on these descriptives.

How to work with a small training data set?

- S-fold cross-validation
  - We create S (equal sized) parts of the training data set.
  - We train using the majority (white) and validate with the withheld (red) data set.
  - We take the average of performance values.
- Extreme case is to have S=N runs, which is also called **leave-one-out**.



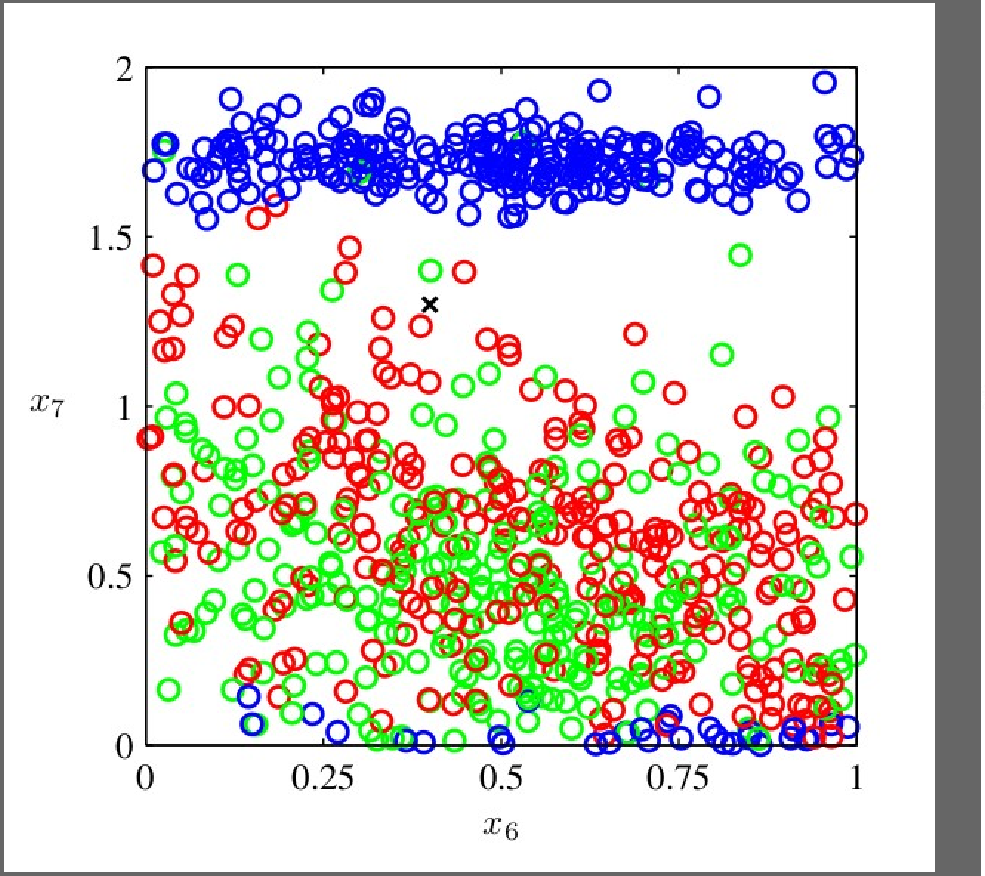
Dimensionality

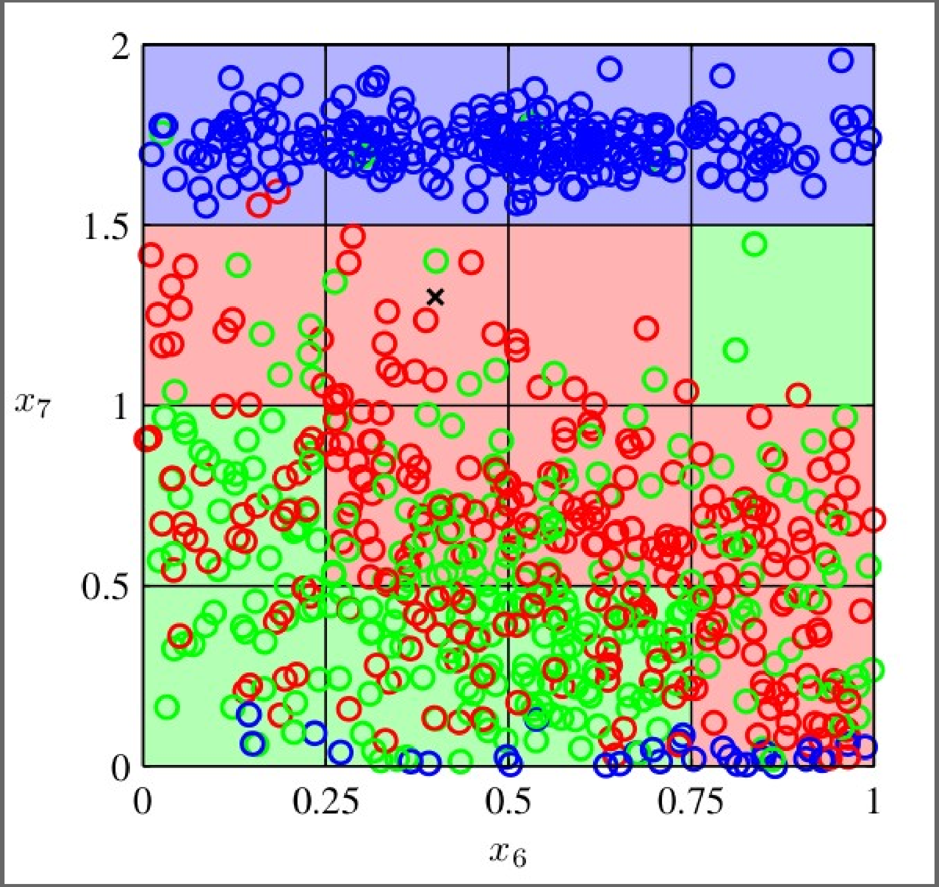
- In our simple example we discussed how we develop a model to **estimate a function of a single variable**.
  - When we have multiple variables (higher dimensionality) this becomes much more complex.

Dimensionality

- We will again use the example from Bishop 2006.
  - The example involves focusing on two variables (out of 12) in a classification problem.
  - The proposed technique divides the space into “zones” which belong to the majority class in the test data set.
  - If a point falls into a zone, then it is classified as from that class.

Dimensionality





Dimensionality

- This approach works “OK” for 3 classes and a 2-dimensional space.
  - How about more classes and the full 12-dimensional space?
  - How many zones do we have? 2^{12}? 3^{12}? 4^{12}?
  - How many coefficients will we need? 12^{2}? 12^{3}? 12^{4}?
- Naive approaches just don’t work with higher dimensions.
  - This is called the **curse of dimensionality** (Bellman, 1961).

Decision Theory and Machine Learning

- Decision theory proposed many methods to make decisions. They usually focus on **optimizing some parameters** in order to:
  - Minimizing false decisions
  - Minimizing expected losses
  - Detecting hard to make decisions

Decision Theory and Machine Learning

- Also consider von Neumann’s minimax theorem and Yao’s principle with multiple turn decision making in a competitive environment.
  - The observations **D** we have on the competitor’s decisions under partially observed environment (test data set) can be used to learn about (ie. estimate a range on) the parameters (**w**), hence **the range of decisions provided by a particular decision making model** we assume she is using.
  - Model selection, parameters as probability distributions, observations as given facts…
  - These are the cornerstones of a Bayesian approach.
  - Bayesian Decision Theory uses machine learning in practical applications.

Model Evaluation Criteria

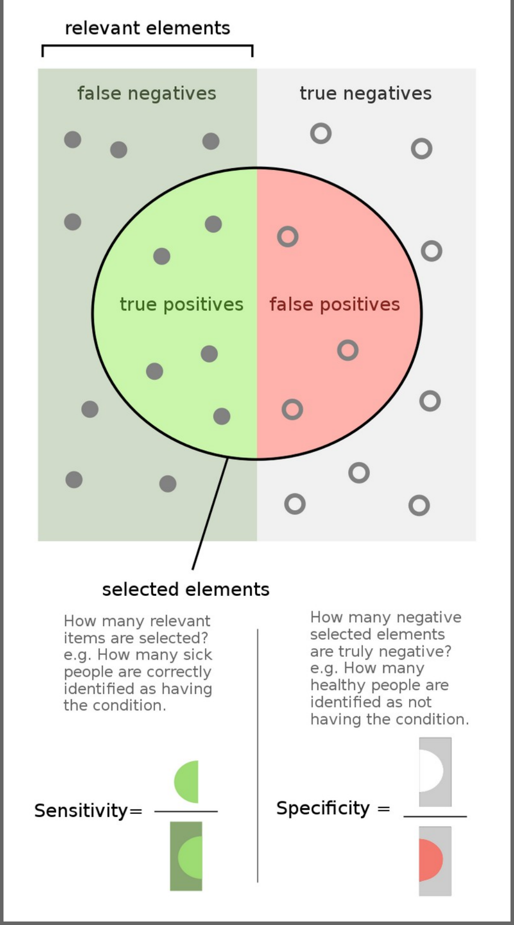
- As we see, we usually design our model prior to training it with the training data set, and then validate it with the validation data set.
  - We should be able to observe problems with the model before we use it in practice.
- Hence we need some model evaluation criteria.

Model Evaluation Criteria

- In classification problems we will have multiple type of problems.
  - The core performance measure, **classification accuracy** is the ratio of correct predictions (tue positives and true negatives) to total predictions made. However in many cases, **error rate** as the rate of all other cases (false negatives, false positives) is also important.
  - In the two-class problem we define the true positive, false positive, true negative, false negative approach easily.

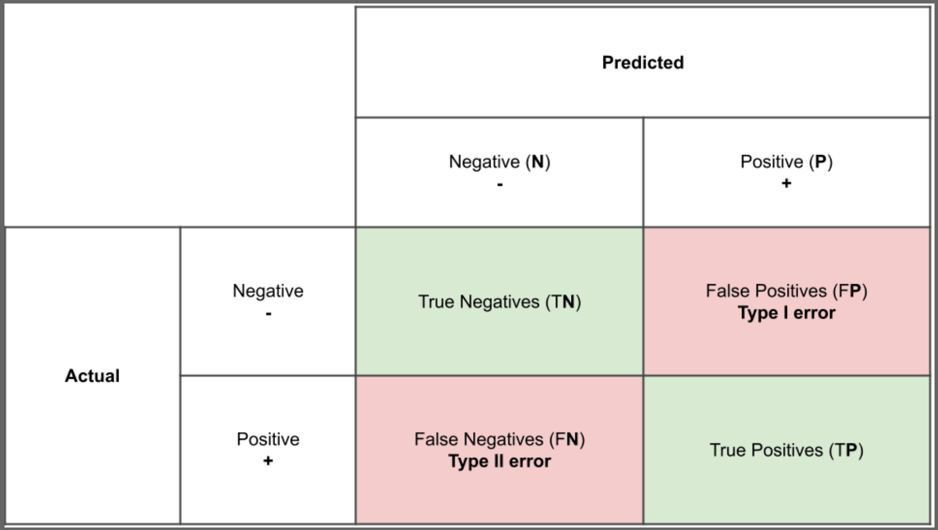
Model Evaluation Criteria

- Sensitivity (recall) and specificity are two important performance criteria we use. (Figure from is from Wikipedia).
  - High sensitivity is always good.
  - High specificity may be more important than high sensitivity because in many applications false positives cause hard to repair damages.


relevant elements
false negatives
true negatives
true positives
false positives
selected elements
How many relevant items are selected? e.g. How many sick people are correctly identified as having the condition.
How many negative selected elements are truly negative? e.g. How many healthy people are identified as not having the condition.
Sensitivity=
Specificity =

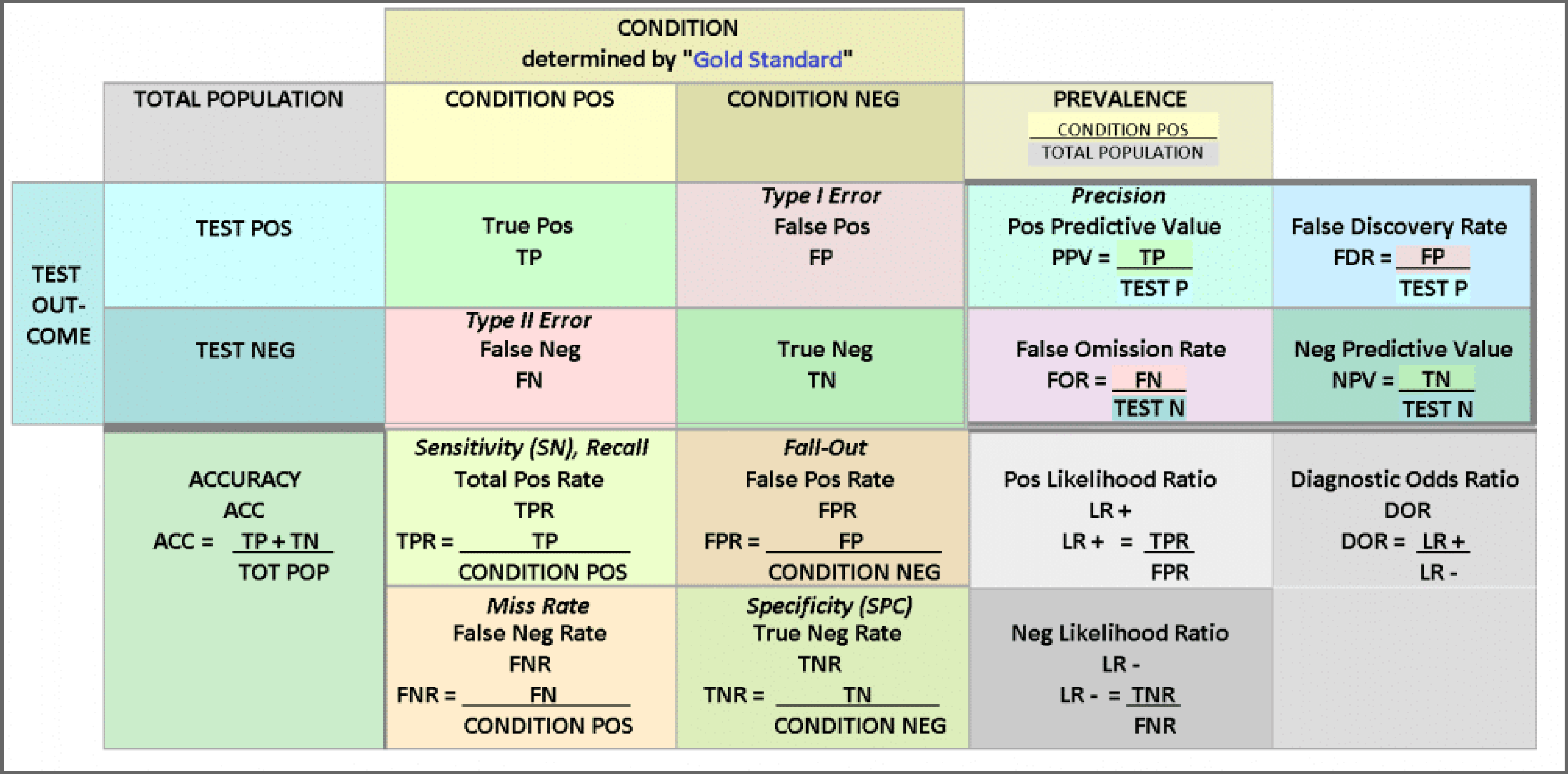
Model Evaluation Criteria

- A confusion matrix is a technique for summarizing the performance of a classification algorithm.
  - We have a series of classifications, actual and predicted and we see their true/false positive/negative nature.
  - We summarize using a matrix.
  - We calculate precision, accuracy and recall.



		Predicted	
		Negative (**N**) **-**	Positive (**P**) **+**
Actual	Negative **-**	True Negatives (T**N**)	False Positives (F**P**) **Type I error**
	Positive **+**	False Negatives (F**N**) **Type II error**	True Positives (T**P**)

Model Evaluation Criteria



		CONDITION determined by "Gold Standard"			
	TOTAL POPULATION	CONDITION POS	CONDITION NEG	PREVALENCE $\frac{\text{CONDITION POS}}{\text{TOTAL POPULATION}}$	
TEST OUT-COME	TEST POS	True Pos TP	*Type I Error* False Pos FP	*Precision* Pos Predictive Value PPV = $\frac{\text{TP}}{\text{TEST P}}$	False Discovery Rate FDR = $\frac{\text{FP}}{\text{TEST P}}$
	TEST NEG	*Type II Error* False Neg FN	True Neg TN	False Omission Rate FOR = $\frac{\text{FN}}{\text{TEST N}}$	Neg Predictive Value NPV = $\frac{\text{TN}}{\text{TEST N}}$
	ACCURACY ACC ACC = $\frac{\text{TP + TN}}{\text{TOT POP}}$	*Sensitivity (SN), Recall* Total Pos Rate TPR TPR = $\frac{\text{TP}}{\text{CONDITION POS}}$	*Fall-Out* False Pos Rate FPR FPR = $\frac{\text{FP}}{\text{CONDITION NEG}}$	Pos Likelihood Ratio LR + LR + = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic Odds Ratio DOR DOR = $\frac{\text{LR +}}{\text{LR -}}$
		Miss Rate False Neg Rate FNR FNR = $\frac{\text{FN}}{\text{CONDITION POS}}$	*Specificity (SPC)* True Neg Rate TNR TNR = $\frac{\text{TN}}{\text{CONDITION NEG}}$	Neg Likelihood Ratio LR - LR - = $\frac{\text{TNR}}{\text{FNR}}$	

Model Evaluation Criteria

- When we have more than 2 classes, calculating TP, TN, etc becomes more complex, but not more difficult.

Model Evaluation Criteria

- R^2 (coefficient of determination) is the proportion of the variation in the dependent variable that is predictable from the independent variable(s).
  - It is used to evaluate the performance of regression based estimation models.
    - An R^2 of 1 indicates that the regression predictions perfectly fit the data.
  - However, a high R^2 can occur in the presence of mis-specification of the functional form of a relationship or in the presence of outliers that distort the true relationship.
  - In many cases SSE (sum of squared errors) is preferred over R^2.

Homework Assignment #2

- Construct a Confusion Matrix based on the classifications made by a hypothetical classifier.
  - You will use the data set provided in the course Github site. The data set has classification results in the validation phase of a 5-class classifier.
  - You will do this by developing code.
    - Submissions in R, Python, Java, etc are accepted.
    - You can also submit a Notebook file.
  - Due Date: March 19th
  - Submission: Through Github.

Questions?

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