Lecture 1: Introduction, Polynomial Curve Fitting, and Probability Theory - 13/01/20

Notations

> using *Classifying Hand Written Digits* as example

- A training set of N digits
- Each digit, i, is an image, representing as an ***input vector of pixel values*** $\boldsymbol{x}_i$
- The category of each digit, i, is known and expresses as ***target vector*** $\boldsymbol{t}_i$
- ML algorithm outputs function $y(\boldsymbol{x})$, which can take new digit input x and output vector y, which is a ***guess*** of the target $\boldsymbol{t}$. The precise form of $y(\boldsymbol{x})$ is determined during the training phases.
- The ability to categorise new examples that differ from those used for training is called ***generalisation***

Supervised Learning

> Problems are ones where the data contains both input and corresponding target vectors.
>
> - ***Classification***
> - ***Regression***

The inputs may be ***pre-processed*** to reduce variability in the inputs.

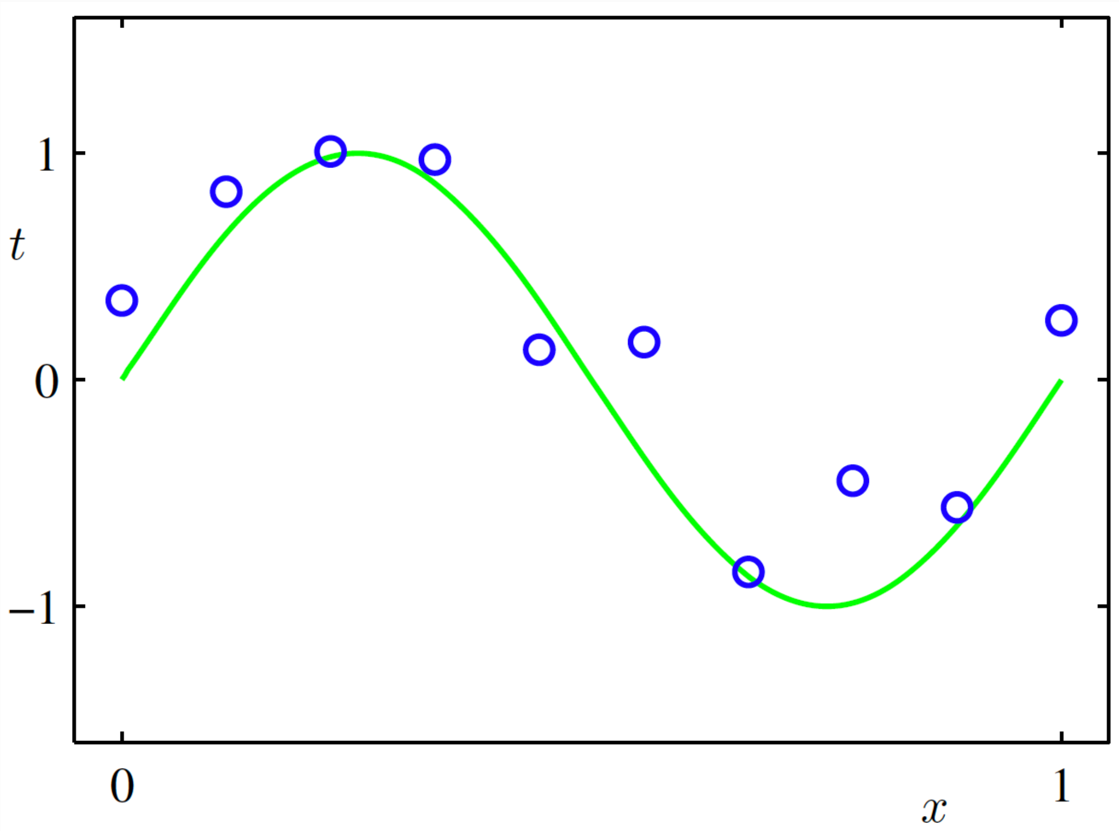
Unsupervised Learning

> Problems are ones where the data contains only input vetors but no targets.
>
> - ***Clustering*** - discovering groups of similiar examples
> - ***Density Estimation*** - learning how data is distributed
> - ***Dimensionality Reduction*** - representing high dimensional data with just a few variables

Reinforcement Learning

> Problems are ones that interact with an environment by choosing actions and observing changes in state. Actions must act to maximise a ***reward signal***. Optimal actions are discovered by ***trials and errors***.

Polynomial Curve Fitting



- ***Training inputs*** $\boldsymbol{x} = (x_1, \dots, x_N)^T$
- ***Training targets*** $\boldsymbol{t} = (t_1, \dots, t_N)^T$

> This is ***synthetic data*** - we know how it originatged

- Each x_i is sampled uniformly from $[0, 1]$
- Each $t_i = sin(2\pi x_i) + (Gaussian\ Noise)$

> Data tends to have an underlying regularity or structure obscured by noise. Noise can be:
>
> - ***intrinsically stochastic*** (random)
> - resulted of ***unobserved*** sources of ***variability***

Aim

- Predict a target $\hat{t}$ for an unseen input $\hat{x}$
- Discover the ***underlying structure***
- Sparate it from the ***noise***

Fitting with Linear Model

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

- M is the ***order of the polynomial***
- ***Polynomial coefficients*** $w_0, \ldots, w_M$ are collected into vector $\mathbf{w}$
- $y(x, \mathbf{w})$ is non-linear in x, but it is linear in $\mathbf{w}$ and so we call this a ***linear model***

> We estimate values for $\boldsymbol{w}$ by fitting the function to training data. Fit the function by ***minising*** an ***error function***

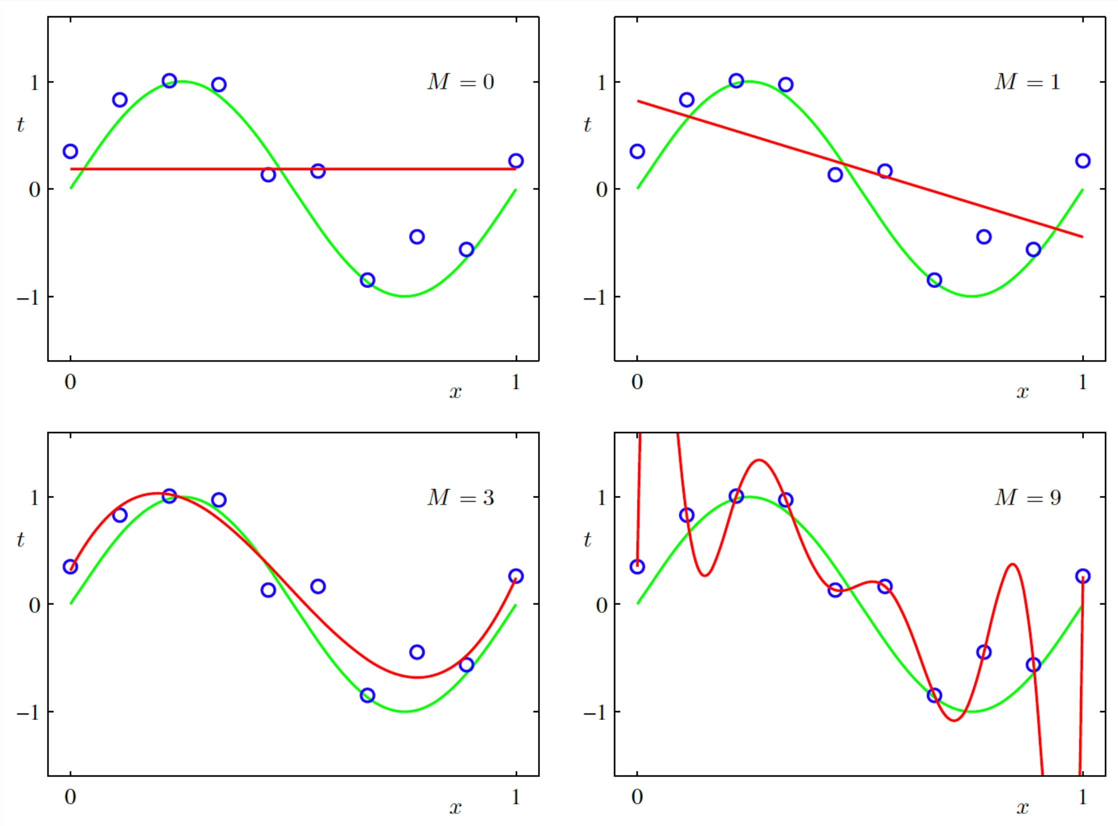
Error Function

A widely used error function is the ***Sum of Square Errors***

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

- ***Best Fit*** $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} E(\mathbf{w})$
- ***Perfect Fit*** if $E(\mathbf{w}^*) = 0$
- Bigger differences are increasingly ***penalised***

Finding the Best Polynomial Degree



> Choosing the best M is an example of ***Model Selection***

> - Small values of M give a poor fit
> - Large values of M appear to ***over-fit*** - ***capture the noise*** rather than underlying structure

Evaluating Fit and Regularisation

We need an objective way to test our fit

Root Mean Squared Error (RMSE)

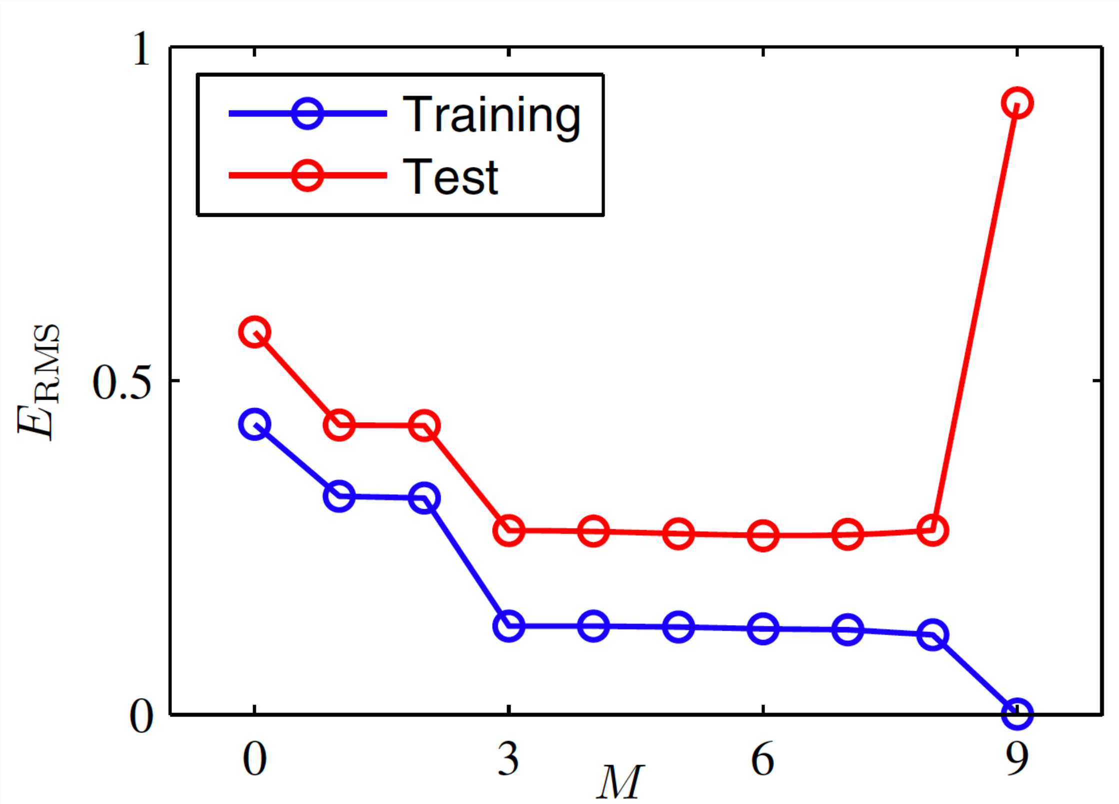
$$E_{RMS} = \sqrt{\frac{2}{N}E(\mathbf{w}^*)}$$

> Comparable for different amounts of data

Avoiding Over-fitting

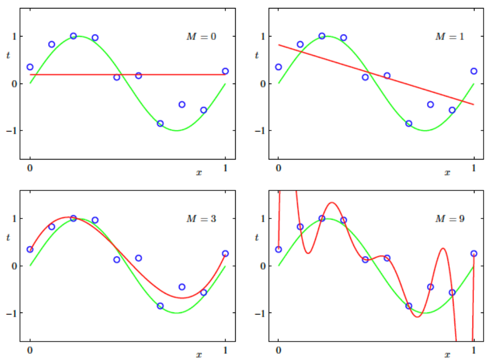
Indirect Evidence of Over-fitting

- Dramatic increse of E_{RMS} of training set and the difference between the E_{RMS} of training set and testing set as degree gets larger
- Magnitude of $\mathbf{w}_i^*$ is extremely large



> Over-fitting means we fail to ***generalise*** to un seen data

	$M=0$	$M=1$	$M=3$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43



> For $M=9$, the magnitude of some $\mathbf{w}_i^*$ are very large, and the model makes some extreme predictions

Dilemma: Complex Models(more expressive) **v.** Over-fitting

Solution 1: Use More Data

Solution 2: Regularisation

Using a new ***error function*** that ***penalises*** extreme parameter values

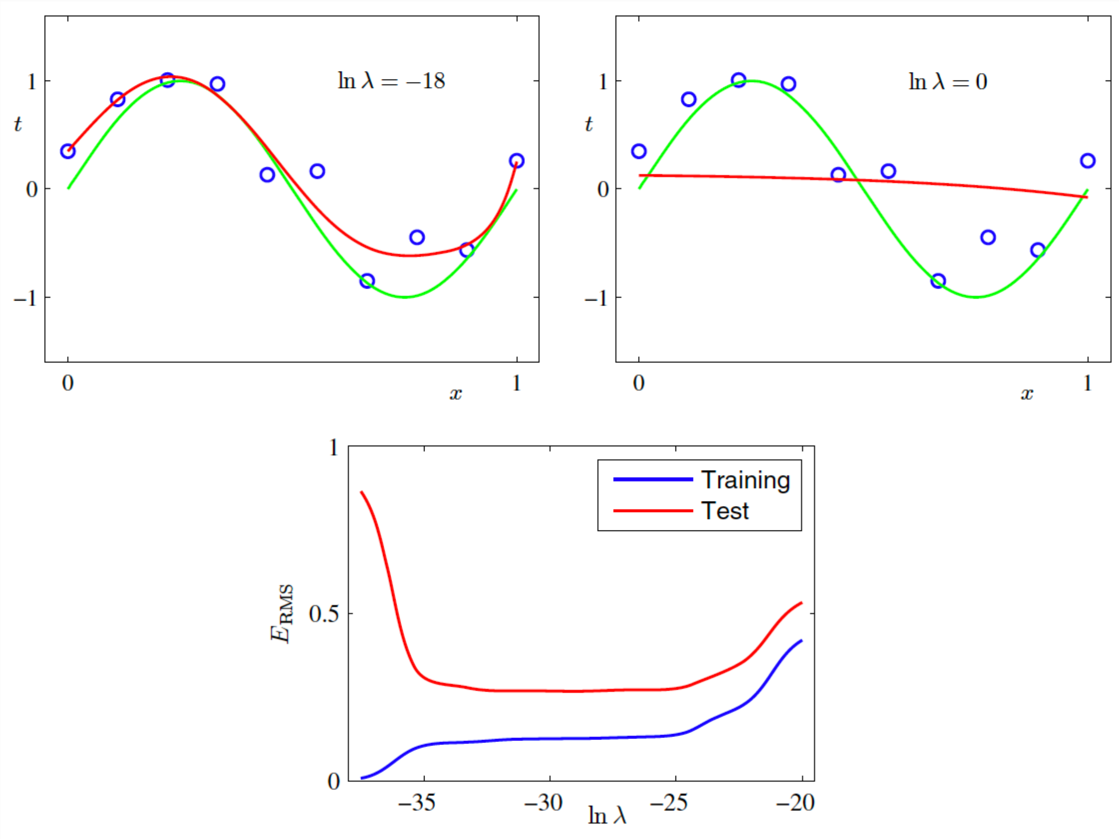
$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}[y(x_n,\mathbf{w}) - t_n]^2 + \frac{\lambda}{2}$$

Where

$$||\mathbf{w}||^2 = \mathbf{w}^T\mathbf{w} = w_0^2 + w_1^2 + \cdots + w_M^2$$

Minimising ***error function***

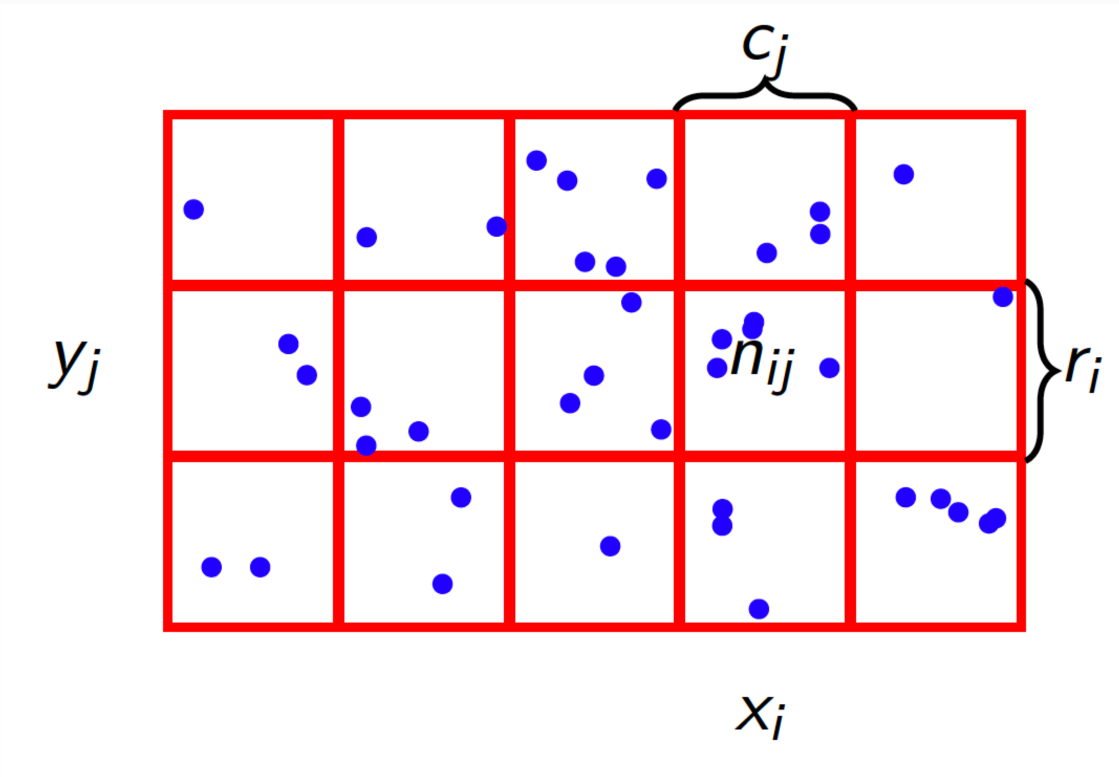
$$\mathbf{w}^* = \arg\min_w \tilde{E}(\mathbf{w})$$



Regularisation appears to control the effective complexity of the model,and hence the degree of overfitting.

Probability Theory

Frequentist Probability



> p_{XY} is ***probability mass function*** over values that random variables X and Y can take.

$$Pr(X = x_i, Y = y_j) = p_{XY}(x_i, y_j)$$

X is a random variable that can take any value x_i, so does Y with y_i

If we sample (X, Y) a large number of times N:

- n_{ij} is the number of times $X = x_i, Y = y_j$
- c_i is the number of times $X = x_i$
- r_j is the number of times $Y = y_j$

> ***Probability mass functions*** capture the relative frequency of outcomes

Probability

Marginal Probability:

$$Pr(X = X_I) = p_X(x_i) = \frac{c_i}{N}$$

Joint Probability:

$$Pr(X = x_i, Y = y_j) = p_{XY}(x_i, y_j) = \frac{n_{ij}}{N}$$

Conditional Probability:

$$Pr(Y = y_j | X = x_i) = p_{Y|X}(y_j|x_i) = \frac{n_{ij}}{c_i}$$

Rule

Sum Rule:

$$p_X(x) = \frac{c_i}{N} = \frac{1}{N}\sum_j n_{ij} = \sum_j p_{xy}(x_i, y_j)$$

Product Rule:

$$p_{XY}(x_i, y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \times \frac{c_i}{N} = p_{Y|X}(y_j|x_i)p_X(x_i)$$

Application in 3 Random Variables Case

$$\begin{aligned} p(x, y) &= \sum_z p(x, y, z) \\ p(x, y, z) &= p(x, y|z)p(z) \\ &= p(y, z|x)p(x) \end{aligned}$$

If $p_{XY}(x, y) = p_X(x)p_Y(y)$, we say X and Y are ***independent***

Application of Probability Rule

Randome Variables:

- ***A*** disease status (***ill*** or ***healthy***)
- ***B*** blood test (***+ve*** or ***-ve***)

$$p_{AB}(a,b) = p_{A|B}(a|b)p_B(b) = p_{B|A}(b|a)p_A(a)$$

$$\begin{aligned}
p_A(ill) &= Pr(person\ has\ disease) = 1\% \\
p_B(+ve) &= Pr(person\ has\ +ve\ blood\ test) = 10\% \\
p_{B|A}(+ve|ill) &= Pr(blood\ test\ is\ +ve\ given\ person\ is\ ill) = 70\% \\
p_{A|B}(ill|+ve) &= Pr(person\ is\ ill\ given\ blood\ test\ is\ +ve) = 7\%
\end{aligned}$$

Reasoning

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

$p(x) = \sum_y p(x|y)p(y)$ ***normalises*** the equation

Practically:

$$\begin{gathered}
p(y|x) \propto p(x|y)p(y) \\
posterior \propto likelihood \times prior
\end{gathered}$$

Frequentist v. Bayesian

> In the frequentist perspective, probability distributions represent ***expected outcomes given a large number of trails***, e.g.
>
> $$E[X] = \lim_{N \to \infty} \frac{1}{N} \sum_n x_n$$

> ***Bayesian Inference*** involves shfting the perspective in order to reason about vents that may ***happen only once***, in which ***probability is a measure of belief***