Statistical Machine Learning

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Outlines

Part II

Introduction to Statistical Machine Learning

Flavour of this course

- Formalise intuitions about problems
- Us
- Ge
- Pro
- Design and analysis of algorithms
- Numerical algorithms in python
- Understand the choices when designing mac
  methods

What is Machine Learning?

Definitio

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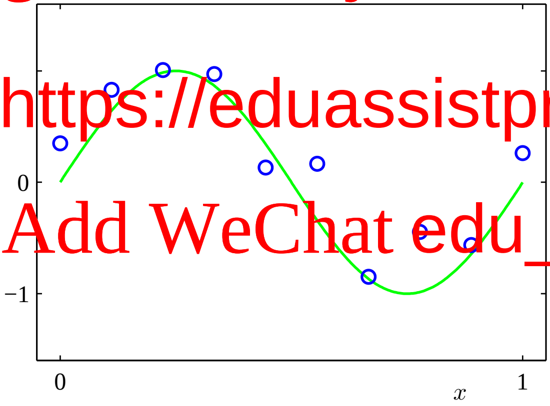
if its perfor
with experience E.

Polynomial Curve Fitting

- some artificial data created from the function

$$\sin(2\pi x) + \text{random noise} \qquad x = 0, \dots, 1$$



Polynomial Curve Fitting - Input Specification

$\equiv ({}_1, \dots, {}_N)$

N

$\mathbf{x}$

$\mathbf{t}$

$x_i \in \mathbb{R} \quad i = 1, \ldots, N$

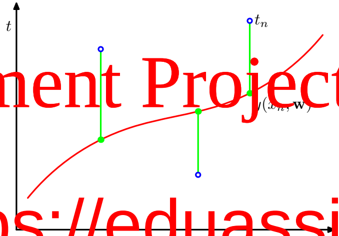
$t_i \in \mathbb{R} \quad i = 1, \ldots, N$

Polynomial Curve Fitting - Model Specification

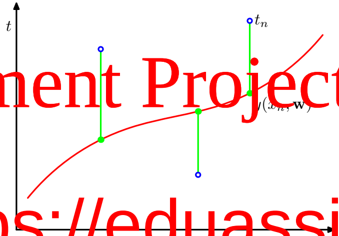
M : order of polynomial

$y(x, \mathbf{w}) =$ ^{2} ^{M}

- nonlinear function of x
- linear function of the unknown model paramet
- How can we find good parameters $\mathbf{w} =$


t
t_n
$y(x_n, \mathbf{w})$

Learning is Improving Performance



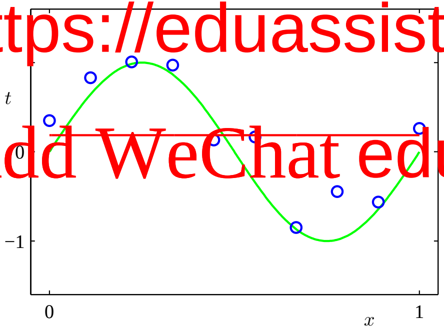
- Performance measure : Error between target prediction of the model for the training data

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

- unique minimum of $E(\mathbf{w})$ for argument $\mathbf{w}^\star$ under certain conditions (what are they?)

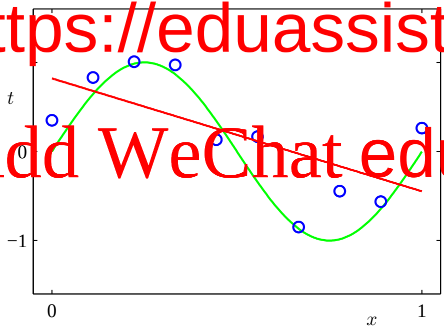
Model Comparison or Model Selection

$$y(x, \mathbf{w}) = \sum_{m=0}^{M} w_m x^m \Bigg|_{M=0}$$



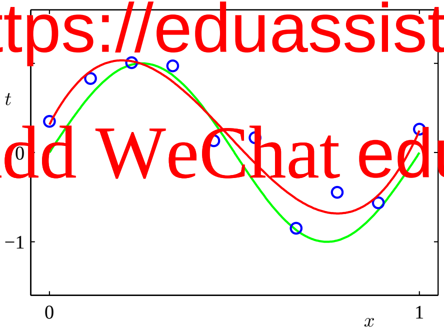
Model Comparison or Model Selection

$$y(x, \mathbf{w}) = \sum_{m=0}^{M} w_m x^m \Bigg|_{M=1}$$



$$y(x, \mathbf{w}) = \sum_{m=0}^{M} w_m x^m \Bigg|_{M=3}$$

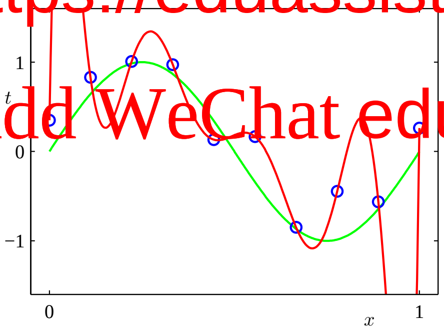
2 3



Model Comparison or Model Selection

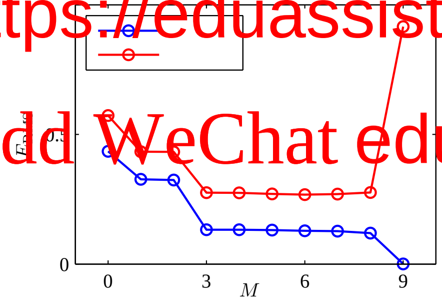
$$
\begin{aligned}
y(x, \mathbf{w}) &= \sum_{m=0}^{M} w_m \, x^m \Bigg|_{M=9} \\
&= w_0 + w_1 \, x + \cdots + w_8 \, x^8 + w_9 \, x^9
\end{aligned}
$$

- ove



Testing the Model

- Train the model and get $\mathbf{w}^\star$
- Get 100 new data points
- Root-mean-square (RMS) error



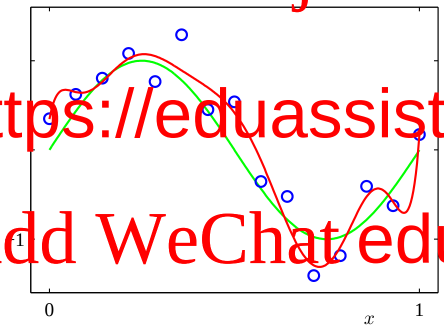
Testing the Model

	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
$w_6^\star$				-1
$w_7^\star$				1
$w_8^\star$				-
$w_9^\star$				

Table: Coefficients $\mathbf{w}^\star$ for polynomials of various order.

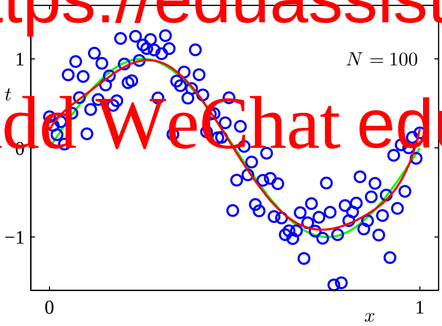
More Data

- $N = 15$



More Data

- $N = 100$
- heuristics : have no less than 5 to 10 times as many data points than parameters
- but number of parameters is not necessarily the most appropriate measure of model complexity !
- late



Regularisation

- How to constrain the growing of the coefficients $\mathbf{w}$?
- Add a regularisation term to the error function

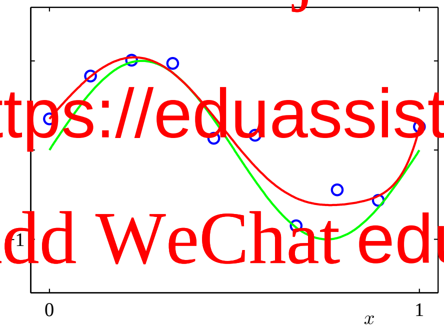
- Squared norm of the parameter vector

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

- unique minimum of $E(\mathbf{w})$ for argument
  conditions (what are they for $\lambda = 0$? for $\lambda > 0$?)

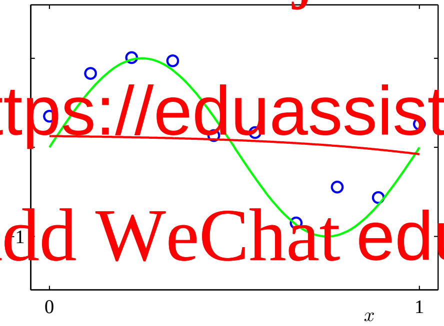
Regularisation

- $M = 9$



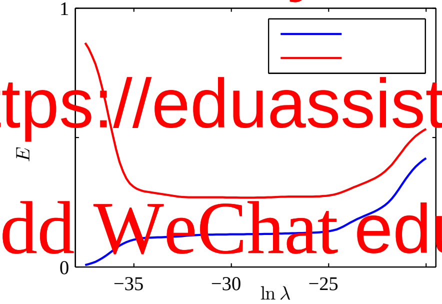
Regularisation

- $M = 9$



Regularisation

- $M = 9$

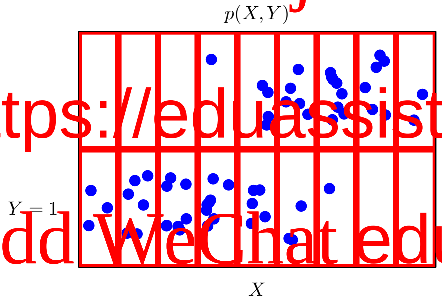


What is Machine Learning?

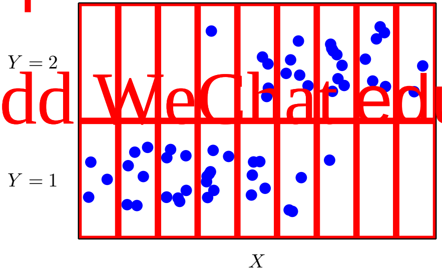
Definition (Mitchell, 1998)

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its perfor
with expe

- Ta
- Experience: $\mathbf{x}$ input examples, $\mathbf{t}$ output l
- Performance: squared error
- Model choice
- Regularisation
- **do not train on the test set!**


$p(X, Y)$
$Y = 1$
X

Y vs. X	a	b	c	d	e	f	g	h	i	sum
2	0	0	0	1	4	5	8	6	2	26
1	3	6	8	8	5	3	1	0	0	34
sum	3	6	8	9	9	8	9	6	2	60



Sum Rule

Y vs. X	a	b	c	d	e	f	g	h	i	sum
2	0	0	0	1	4	5	8	6	2	26
1	3	6	8	8	5	3	1	0	0	34
sum	3	6	8	9	9	8	9	6	2	60

$p($

$$= 1/60 + 8/60$$

$$p(X = d) = \sum_Y p(X = d,$$

$$p(X) = \sum_Y p(X, Y)$$

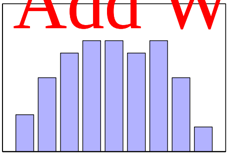
Sum Rule

Y vs. X	a	b	c	d	e	f	g	h	i	sum
2	0	0	0	1	4	5	8	6	2	26
1	3	6	8	8	5	3	1	0	0	34
sum	3	6	8	9	9	8	9	6	2	60

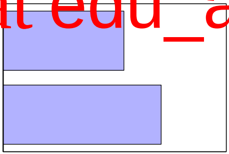
p

Y X

$p(X)$



X



Product Rule

Y vs. X	a	b	c	d	e	f	g	h	i	sum
2	0	0	0	1	4	5	8	6	2	26
1	3	6	8	8	5	3	1	0	0	34
sum	3	6	8	9	9	8	9	6	2	60

Conditional Probability

Calculat

$$p(Y = 1) = \sum_X p(X, Y = 1) =$$

$$p(X = d, Y = 1) = p(X = d \mid Y =$$

$$p(X, Y) = p(X \mid Y)\, p(Y)$$

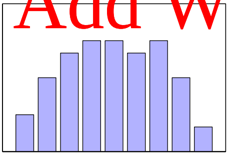
Another intuitive view is renormalisation of relative frequencies:

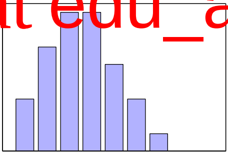
$$p(X \mid Y) = \frac{p(X, Y)}{p(Y)}$$

Y vs. X	a	b	c	d	e	f	g	h	i	sum
2	0	0	0	1	4	5	8	6	2	26
1	3	6	8	8	5	3	1	0	0	34
sum	3	6	8	9	9	8	9	6	2	60

p ... Y

$p(X)$





Sum Rule and Product Rule

- Sum Rule

- Pro

These rules form the basis of Bayesian machine lear
this course!

Bayes Theorem

Use product rule

$$p(X, Y) = p(X \mid Y)\, p(Y) = p(Y \mid X)\, p(X)$$

Bayes Theorem

$$p(Y \mid X) = \frac{p(X \mid Y)\, p(Y)}{p(X)}$$

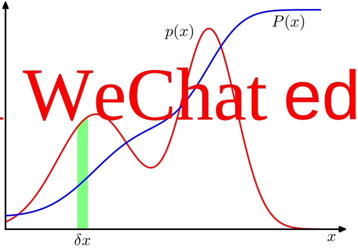
and

$$p(X) = \sum_Y p(X, Y)$$

$$= \sum_Y p(X \mid Y)\, p(Y) \qquad \text{(product rule)}$$

Probability Densities

- Real valued variable $x \in \mathbb{R}$
- Probability of x to fall in the interval $(x, x + \delta x)$ is given by $p(x)\delta x$ for infinitesimal small δx.
-

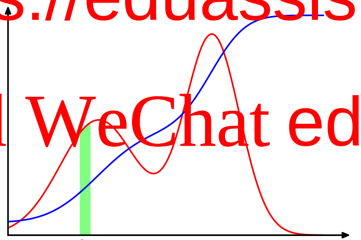


Constraints on $p(x)$

- Nonnegative

$$p(x) \geq 0$$

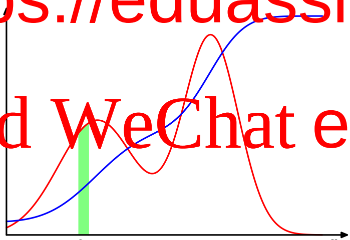
- Normalisation



Cumulative distribution function $P(x)$

$$P(x) = \int_{-\infty}^{x} p(z)\, \mathrm{d}z$$

or



Multivariate Probability Density

- Vector $\mathbf{x} \equiv (x_1, \dots, x_D)^T = \begin{bmatrix} x_1 \\ \vdots \\ x_D \end{bmatrix}$
- No
- Nor

$$\int_{-\infty}^{\infty} p(\mathbf{x})\,\mathrm{d}\mathbf{x} = 1.$$

- This means

$$\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} p(\mathbf{x})\,\mathrm{d}x_1 \dots \mathrm{d}x_D = 1.$$

- Su

- Pro

$$p(x, y) = p(y \mid x)\, p(x$$

Expectations

- Weighted average of a function f(x) under the probability dist

$$\mathbb{E}\left[f\right] = \int p(x)\, f(x)\, \mathrm{d}x$$ proba

How to approximate $\mathbb{E}[f]$

- Given a finite number N of points x_n drawn from the probability distribution $p(x)$.
- Ap

$$\simeq \frac{1}{N}\sum_{n=1}^{N} f(x_n)$$

- How to draw points from a probability distribution? Lecture coming about "Sampling"

Expection of a function of several variables

- arbitrary function $f(x, y)$

$\mathbb{E}_x$

$$\mathbb{E}_x [f(x, y)] = \quad p(x) f(x, y)\, \mathrm{d}x$$ probability density $p(x)$

- Note that $\mathbb{E}_x [f(x, y)]$ is a function of y.

Conditional Expectation

- arbitrary function $f(x)$

$$\mathbb{E}_x[f \mid y] = \sum_x p(x \mid y)\, f(x) \qquad \text{discrete distribution } p(x)$$

$$\mathbb{E}_x[f \mid y] = \quad p(x \mid y)\, f(x)\, \mathrm{d}x \qquad \text{probability density } p(x)$$

- Not
- Oth
- Wh $[\;[\;(\;)\;|\;]]$

- This must mean $\mathbb{E}_y[\mathbb{E}_x[f(x) \mid y]]$. (Why?)

$$\begin{aligned}\mathbb{E}_y[\mathbb{E}_x[f(x) \mid y]] &= \sum_y p(y)\, \mathbb{E}_x[f \mid y] = \\ &= \sum_{x,y} f(x)\, p(x,y) = \sum_x f(x)\, p(x) \\ &= \mathbb{E}_x[f(x)]\end{aligned}$$

Variance

- arbitrary function $f(x)$

- Sp

$$\operatorname{var}[x] = \mathbb{E}\left[(x - \mathbb{E}[x])^2\right] = \mathbb{E}\left[\right.$$

Covariance

- Two random variables $x \in \mathbb{R}$ and $y \in \mathbb{R}$

$$\operatorname{cov}[x, y] = \mathbb{E}_{x,y}\left[(x - \mathbb{E}[x])(y - \mathbb{E}[y])\right]$$
$$= \mathbb{E}_{x,y}[x\,y] - \mathbb{E}[x]\,\mathbb{E}[y]$$

- Wit

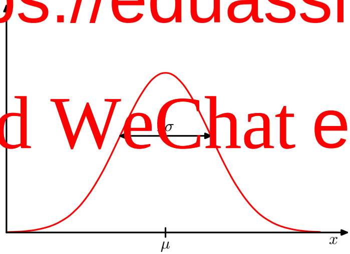
$$= {}_{x,y}[\quad] - {}_{x,y}[\quad] - {}_{x,y}[\quad] + {}_{x,y}[\quad]$$
$$= \mathbb{E}_{x,y}[x\,y] - b\,\underbrace{\mathbb{E}_{x,y}[x]}_{=\mathbb{E}_x[x]} - a\,\mathbb{E}$$
$$= \mathbb{E}_{x,y}[x\,y] - a\,b - a\,b + a\,b \qquad {}_{x,y}$$
$$= \mathbb{E}_{x,y}[x\,y] - \mathbb{E}[x]\,\mathbb{E}[y]$$

- Expresses how strongly x and y vary together. If x and y are independent, their covariance vanishes.

- Tw

$$= \mathbb{E}_{\mathbf{x},\mathbf{y}} \quad \mathbf{x}\,\mathbf{y} \quad - \mathbb{E}\left[\mathbf{x}\right]\mathbb{E} \quad \mathbf{y}$$

- $x \in \mathbb{R}$
- Gaussian Distribution with mean μ and variance σ^2



The Gaussian Distribution

- $\mathcal{N}(x \,|\, \mu, \sigma^2) > 0$
- $\int_{-\infty}^{\infty} \mathcal{N}(x \,|\, \mu, \sigma^2) \,\mathrm{d}x = 1$
- Expectation over x

- Exp

$$\mathbb{E}\left[x^2\right] = \int_{-\infty}^{\infty} \mathcal{N}(x \,|\, \mu, \sigma^2)\, x^2 \,\mathrm{d}x$$

- Variance of x

$$\operatorname{var}[x] = \mathbb{E}\left[x^2\right] - \mathbb{E}\left[x\right]^2 = \sigma^2$$

Strategy in this course

- Estimate best predictor = training = learning
  Giv

  1.
  2.
  3.
  4. Calculate the optimal parameter ($\mathbf{w}$)
  5. Model uncertainty using the Bayesian appro
  6. Implement and compute (the algorithm in py
  7. Interpret and diagnose results