Statistical Machine Learning

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

Outlines

Part II

Introduction

Flavour of this course

- Formalise intuitions about problems
- Use language of mathematics to express models
- Geometry, vectors, linear algebra for reasoning
- Probabilistic models to capture uncertainty
- Design and analysis of algorithms
- Numerical algorithms in python
- Understand the choices when designing machine learning methods

What is Machine Learning?

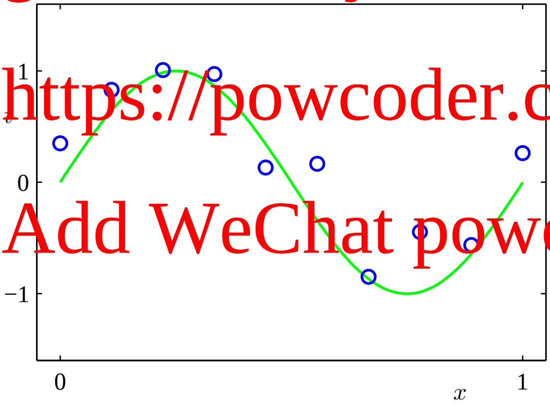
Definition (Mitchell, 1998)

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

Polynomial Curve Fitting

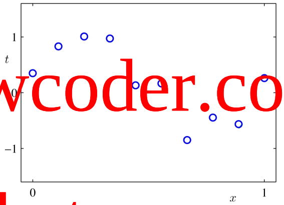
- some artificial data created from the function

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



Polynomial Curve Fitting - Input Specification

$$N = 10$$
$$\mathbf{x} \equiv (x_1, \dots, x_N)^T$$
$$\mathbf{t} \equiv (t_1, \dots, t_N)^T$$



Polynomial Curve Fitting - Input Specification

$$N = 10$$

$$\mathbf{x} \equiv (x_1, \dots, x_N)^T$$

$$\mathbf{t} \equiv (t_1, \dots, t_N)^T$$

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

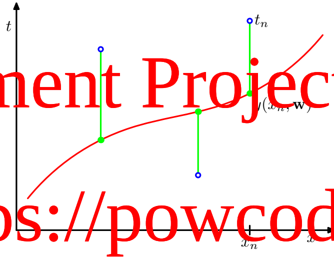
$$t_i \in \mathbb{R} \quad i = 1, \dots, N$$

Polynomial Curve Fitting - Model Specification

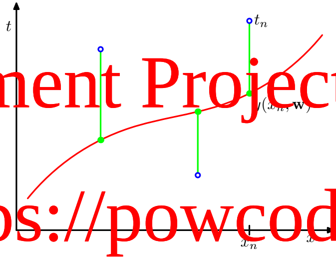
M : order of polynomial

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

- nonlinear function of x
- linear function of the unknown model parameter $\mathbf{w}$
- How can we find good parameters $\mathbf{w} = (w_1, \dots, w_M)^T$?


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

Learning is Improving Performance



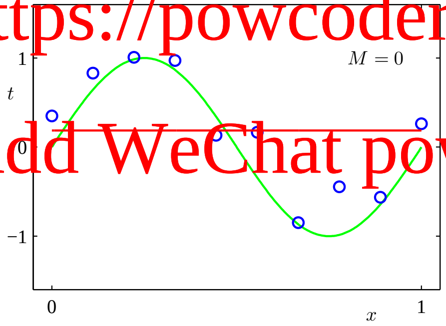
- Performance measure : Error between target and prediction of the model for the training data

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

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

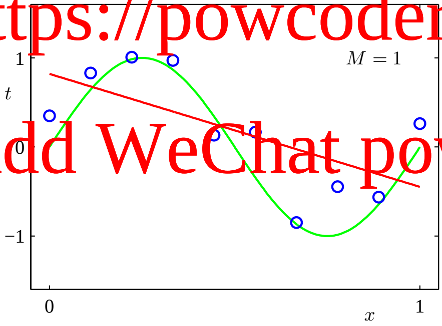
Model Comparison or Model Selection

$$y(x, \mathbf{w}) = \sum_{m=0}^{M} w_m x^m \Big|_{M=0} = w_0$$



Model Comparison or Model Selection

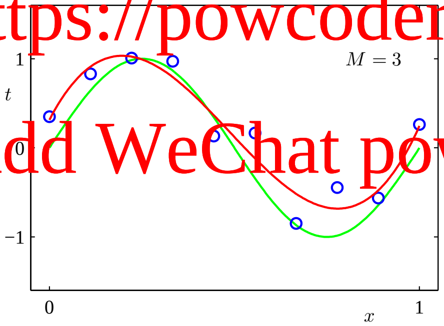
$$
\begin{aligned}
y(x, \mathbf{w}) &= \sum_{m=0}^{M} w_m x^m \Bigg|_{M=1} \\
&= w_0 + w_1 x
\end{aligned}
$$



Model Comparison or Model Selection

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

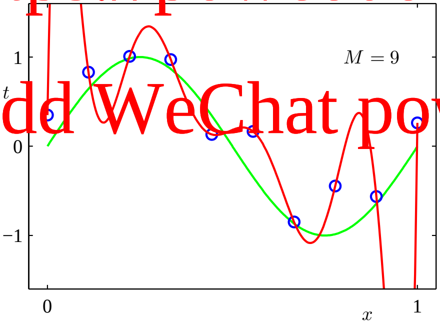
$$
= w_0 + w_1 x + w_2 x^2 + w_3 x^3
$$



Model Comparison or Model Selection

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

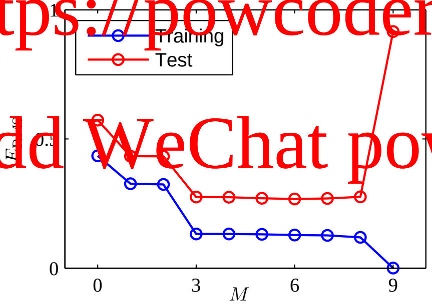
- over-fitting



Testing the Model

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

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



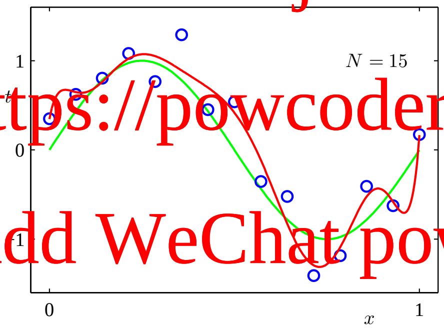
Testing the Model

	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
$w_2^\star$			-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

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

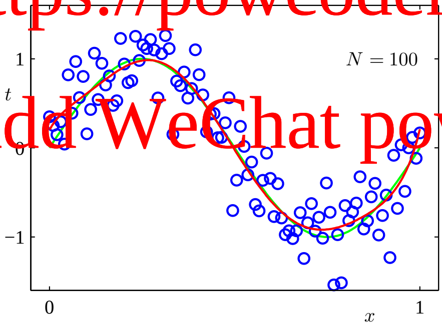
More Data

- $N = 15$



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 !
- later: Bayesian approach



Regularisation

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

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

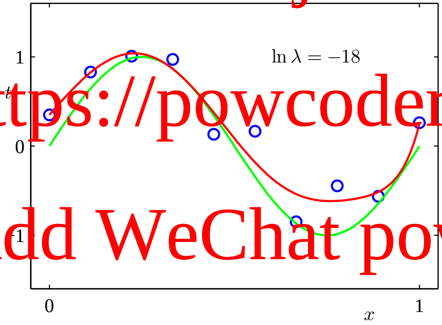
- Squared norm of the parameter vector $\mathbf{w}$

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

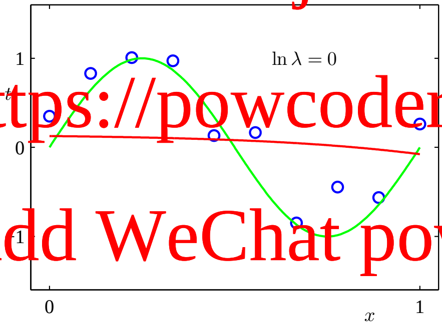
- unique minimum of $E(\mathbf{w})$ for argument $\mathbf{w}^\star$ under certain conditions (what are they for $\lambda = 0$? for $\lambda > 0$?)

Regularisation

- $M = 9$

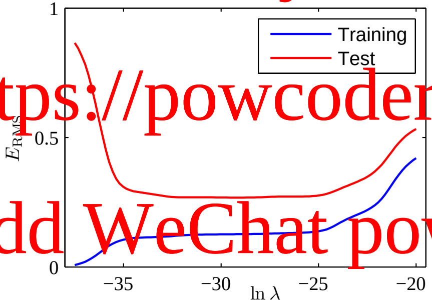


- $M = 9$



Regularisation

- $M = 9$

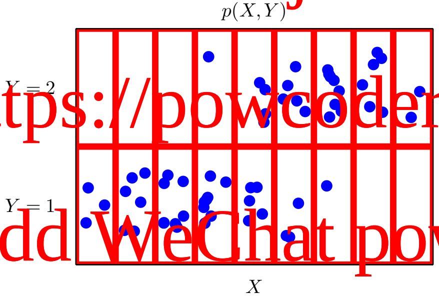


What is Machine Learning?

Definition (Mitchell, 1998)

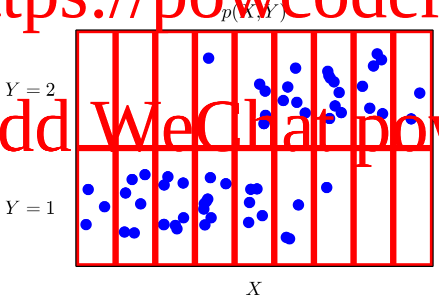
A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

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


$p(X, Y)$
$Y = 2$
$Y = 1$
X

Probability Theory

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

$$p(X = d, Y = 1) = 8/60$$

$$p(X = d) = p(X = d, Y = 2) + p(X = d, Y = 1)$$
$$= 1/60 + 8/60$$

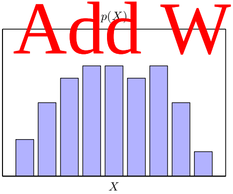
$$p(X = d) = \sum_Y p(X = d, Y)$$

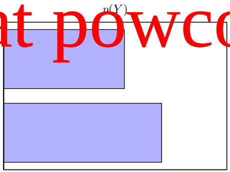
$$p(X) = \sum_Y p(X, Y)$$

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

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





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

$$p(X = d \mid Y = 1) = 8/34$$

Calculate $p(Y = 1)$:

$$p(Y = 1) = \sum_X p(X, Y = 1) = 34/60$$

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

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

Another intuitive view is renormalisation of relative frequencies:

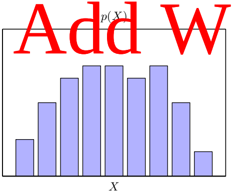
$$p(X \mid Y) = \frac{p(X, Y)}{p(Y)}$$

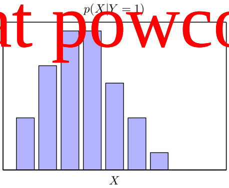
Sum and Product Rules

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

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

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





Sum Rule and Product Rule

- Sum Rule

$$p(X) = \sum_{Y} p(X, Y)$$

- Product Rule

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

These rules form the basis of Bayesian machine learning, and this course!

Bayes Theorem

Use product rule

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

Bayes Theorem

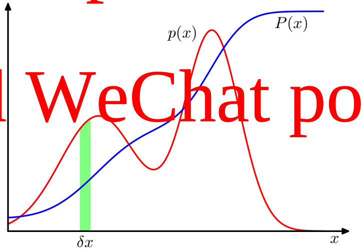
$$p(Y \mid X) = \frac{p(X \mid Y)\, p(Y)}{p(X)} \qquad \text{only defined for } p(X) > 0$$

and

$$\begin{aligned} p(X) &= \sum_Y p(X, Y) && \text{(sum rule)} \\ &= \sum_Y p(X \mid Y)\, p(Y) && \text{(product rule)} \end{aligned}$$

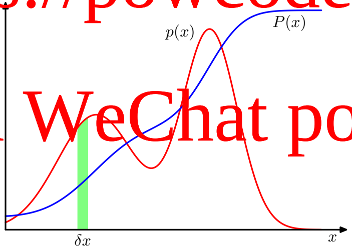
Probability Densities

- 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.
- $$p(x \in (a, b)) = \int_a^b p(x) \, \mathrm{d}x.$$



Constraints on $p(x)$

- Nonnegative
$$p(x) \geq 0$$
- Normalisation
$$\int_{-\infty}^{\infty} p(x) \, \mathrm{d}x = 1.$$

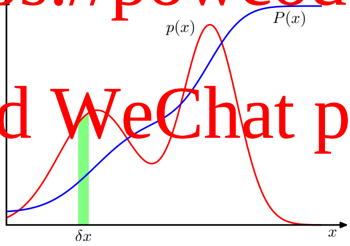


Cumulative distribution function $P(x)$

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

or

$$\frac{d}{dx} P(x) = p(x)$$



- Vector $\mathbf{x} \equiv (x_1, \dots, x_D)^T = \begin{bmatrix} x_1 \\ \vdots \\ x_D \end{bmatrix}$

- Nonnegative

$$p(\mathbf{x}) \geq 0$$

- Normalisation

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

- This means

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

Sum and Product Rule for Probability Densities

- Sum Rule

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

- Product Rule

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

Expectations

- Weighted average of a function f(x) under the probability distribution $p(x)$

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

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

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

- Given a finite number N of points x_n drawn from the probability distribution $p(x)$.
- Approximate the expectation by a finite sum:

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

- How to draw points from a probability distribution $p(x)$? Lecture coming about “Sampling”

Expection of a function of several variables

- arbitrary function $f(x, y)$

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

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

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

Conditional Expectation

- arbitrary function $f(x)$

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

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

- Note that $\mathbb{E}_x[f \mid y]$ is a function of y.
- Other notation used in the literature : $\mathbb{E}_{x|y}[f]$.
- What is $\mathbb{E}[\mathbb{E}[f(x) \mid y]]$? Can we simplify it?
- This must mean $\mathbb{E}_y[\mathbb{E}_x[f(x) \mid y]]$. (Why?)

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

Variance

- arbitrary function $f(x)$

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

- Special case: $f(x) = x$

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

Covariance

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

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

- With $\mathbb{E}[x] = a$ and $\mathbb{E}[y] = b$

$$
\begin{aligned}
\operatorname{cov}[x, y] &= \mathbb{E}_{x,y}\left[(x - a)(y - b)\right] \\
&= \mathbb{E}_{x,y}[x\,y] - \mathbb{E}_{x,y}[x\,b] - \mathbb{E}_{x,y}[a\,y] + \mathbb{E}_{x,y}[a\,b] \\
&= \mathbb{E}_{x,y}[x\,y] - b\,\underbrace{\mathbb{E}_{x,y}[x]}_{=\mathbb{E}_x[x]} - a\,\underbrace{\mathbb{E}_{x,y}[y]}_{=\mathbb{E}_y[y]} + a\,b\,\underbrace{\mathbb{E}_{x,y}[1]}_{=1} \\
&= \mathbb{E}_{x,y}[x\,y] - a\,b - a\,b + a\,b = \mathbb{E}_{x,y}[x\,y] - a\,b \\
&= \mathbb{E}_{x,y}[x\,y] - \mathbb{E}[x]\,\mathbb{E}[y]
\end{aligned}
$$

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

Covariance for Vector Valued Variables

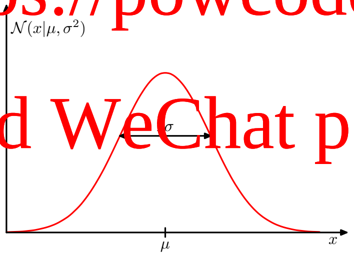
- Two random variables $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{y} \in \mathbb{R}^D$

$$\begin{aligned} \operatorname{cov}[\mathbf{x}, \mathbf{y}] &= \mathbb{E}_{\mathbf{x},\mathbf{y}}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{y}^{\mathbf{T}} - \mathbb{E}[\mathbf{y}^{\mathbf{T}}])\right] \\ &= \mathbb{E}_{\mathbf{x},\mathbf{y}}\left[\mathbf{x}\,\mathbf{y}^{\mathbf{T}}\right] - \mathbb{E}[\mathbf{x}]\,\mathbb{E}\left[\mathbf{y}^{\mathbf{T}}\right] \end{aligned}$$

The Gaussian Distribution

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

$$\mathcal{N}(x \mid \mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\}$$



The Gaussian Distribution

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

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}(x \mid \mu, \sigma^2) \, x \, dx = \mu$$

- Expectation over x^2

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} \mathcal{N}(x \mid \mu, \sigma^2) \, x^2 \, dx = \mu^2 + \sigma^2$$

- Variance of x

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

Strategy in this course

- Estimate best predictor = training = learning
  Given data $(x_1, y_1), \dots, (x_n, y_n)$, find a predictor $f_{\mathbf{w}}(\cdot)$.

  1. Identify the type of input x and output y data
  2. Propose a (linear) mathematical model for $f_{\mathbf{w}}$
  3. Design an objective function or likelihood
  4. Calculate the optimal parameter ($\mathbf{w}$)
  5. Model uncertainty using the Bayesian approach
  6. Implement and compute (the algorithm in python)
  7. Interpret and diagnose results