# CS5014 Machine Learning

Lecture 2 Maths background review

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# So why this review session?

#### Maths is useful

- rigorous and concise way of communicating results
- help us understand why and why not algorithms work
- be able to derive your own model and algorithms!

#### Refresher on essential concepts

- only a refresher; we expect you have learnt them
  - don't expect to know everything after this lecture
- not complete and not rigorous

#### Self-assessment for yourself

- identify rusty area
- do self studies afterwards
- maths learning should be never-ending :-)

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# Mathematics for machine learning

#### Linear algebra

- leap forward from elementary algebra: 1-d to multi-dimensional
- number line to a number plane (space)

### Probability theory and statistics

- study of uncertainty: uncertainty is the norm
  - e.g. rain tomorrow? blood pressure measurement (reading error)?
- how to generalise your results
  - from one sample to the universe: vaccine trial

- study of continuous (real-valued) functions (using approximation, say polynomial)
  - y = sin(x) is well approximated by y = x when  $x \approx 0$
- useful when we do optimisation

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# Useful textbook and references (read the italic entries!)

#### Linear algebra

- Learning from Data Supplementary Mathematics (Vector and Linear Algebra) by David Barber;
   https://api.semanticscholar.org/CorpusID:18857001
- Chapter 2 of Deep Learning by Ian Goodfellow, Yoshua Bengio and Aaron Courville https://www.deeplearningbook.org/contents/linear\_algebra.html
- Introduction to Linear Algebra by Gilbert Strang; http://math.mit.edu/~gs/linearalgebra/
- The Matrix Cookbook by Kaare Brandt Petersen, Michael Syskind Pedersen;
  - https://www2.imm.dtu.dk/pubdb/pubs/3274-full.html
    - useful as a reference manual

#### Probability theory

- Chapter 2.1-2.3 Information Theory, Inference, and Learning Algorithms by David J.C. MacKay http://www.inference.org.uk/itprnn/book.pdf
- Chapter 3.1-3.9 of Deep Learning by Ian Goodfellow, Yoshua Bengio and Aaron Courville https://www.deeplearningbook.org/contents/prob.html
- Introduction to Probability Models by Sheldon Ross
  - chapter 1; chapter 2.1-2.5, 2.8; chapter 3.1-3.5

- Use your book of choice; read multivariate calculus part as well
- Appendix of Bayesian Reasoning and Machine Learning by David Barber
  - http://web4.cs.ucl.ac.uk/staff/D.Barber/textbook/200620.pdf

### Linear algebra: Basic concepts

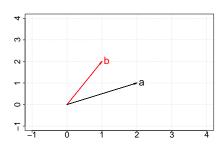
- vectors
- norms and distances
- linear independence, span, subspace
- matrices, linear transformation
- matrix operations
- rank

#### Vector

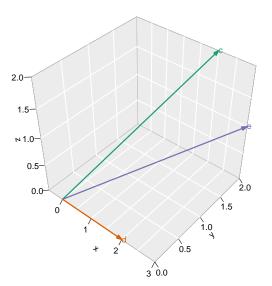
#### A vector is a collection of n salars

- $a \in \mathbb{R}^n$ , default option is column vector i.e.  $n \times 1$
- represents a **displacement** in R<sup>n</sup>

• e.g. 
$$\mathbf{a} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$
 (or  $\mathbf{a} = [2, 1]^T$  to save space)



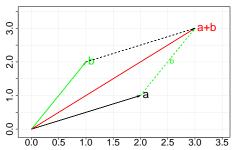
Some 3-d vectors 
$$\mathbf{c} = \begin{bmatrix} 2 \\ 2 \\ 2 \end{bmatrix}$$
,  $\mathbf{d} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$ ,  $\mathbf{e} = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$ 



#### Vector addition

$$m{a} + m{b} = egin{bmatrix} a_1 \ a_2 \ dots \ a_d \end{bmatrix} + egin{bmatrix} b_1 \ b_2 \ dots \ b_d \end{bmatrix} = egin{bmatrix} a_1 + b_1 \ a_2 + b_2 \ dots \ a_d + b_d \end{bmatrix}$$

- generalisation from scalar arithmetics; remember 2+1 on a number axis?
- parallelogram rule



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### Vector scaling/multiplication

$$k \cdot \mathbf{a} = k \cdot \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_d \end{bmatrix} = \begin{bmatrix} k \times a_1 \\ k \times a_2 \\ \vdots \\ k \times a_d \end{bmatrix}, k \in R \text{ or a scalar}$$

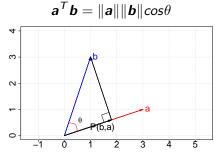
- geometrically, scaling means shrinking or streching a vector
  - the direction does not change but length changes
- and obviously  $n \cdot a = a + \ldots + a = \sum_{n} a$
- $\bullet$   $0 \cdot a = 0$ က  $\alpha$

### Inner product

$$\boldsymbol{a}^{T}\boldsymbol{b} = [a_1, a_2 \dots, a_d] \cdot \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_d \end{bmatrix} = \sum_{i=1}^{d} a_i \times b_i$$

- $a^T b = b^T a$  and the result is a scalar
- $a^T(b+c) = a^Tb + a^Tc$
- $(k\mathbf{a})^T\mathbf{b} = \mathbf{a}^T(k\mathbf{b}) = k(\mathbf{a}^T\mathbf{b})$
- $a^Ta = \sum_{i=1}^d a_i^2$  is squared Euclidean distance between a and 0
- $\mathbf{a}^T \mathbf{a} \geq 0$  and  $\mathbf{a} = \mathbf{0}$  if and only if  $\mathbf{a}^T \mathbf{a} = 0$

#### Another interpretation:



- $\theta$  is the angle between a, b
  - $\mathbf{a}^T \mathbf{b} = 0$  if and only if  $\mathbf{a} \perp \mathbf{b}$
- $\|a\|\cos\theta$  is the projected length of **a** on **b**
- $\| \boldsymbol{b} \| \cos \theta$  is the projected length of  $\boldsymbol{b}$  on  $\boldsymbol{a}$
- $P(\mathbf{b}, \mathbf{a})$  denotes the projected vector of  $\mathbf{b}$  to  $\mathbf{a}$ 
  - so  $\|\boldsymbol{b}\|\cos\theta = \|P(\boldsymbol{b},\boldsymbol{a})\|$
- and (prove it or convince yourself!)

$$P(\boldsymbol{b}, \boldsymbol{a}) = \|\boldsymbol{b}\|\cos\theta * \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} = \frac{\boldsymbol{a}^T\boldsymbol{b}}{\boldsymbol{a}^T\boldsymbol{a}}\boldsymbol{a}$$

### Matrix

A rectangular array of real numbers  $A \in R^{m \times n}$ 

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \mathbf{a}_{1} & \mathbf{a}_{2} & \dots & \mathbf{a}_{n} \\ | & | & & | \end{bmatrix} = \begin{bmatrix} - & \tilde{\mathbf{a}}_{1} & - \\ \vdots & \vdots & \vdots \\ - & \tilde{\mathbf{a}}_{m} & - \end{bmatrix}$$

- can be viewed as a collection of n column vectors
  - $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n];$
- or row vectors  $\mathbf{A} = [\mathbf{\tilde{a}}_1^T, \mathbf{\tilde{a}}_2^T, \dots, \mathbf{\tilde{a}}_m^T]^T$
- sometimes written as  $\mathbf{A} = (a_{ij})$   $i = 1, \dots, m, j = 1, \dots, n$

# Matrix operations

- addition:  $\mathbf{A} + \mathbf{B} = \mathbf{C} = (c_{ij})$  where  $c_{ij} = a_{ij} + b_{ij}$
- scaling:  $k\mathbf{A} = \mathbf{C}$  where  $c_{ij} = k * a_{ij}$
- transpose:  $\boldsymbol{A}^T = \boldsymbol{C}$  where  $c_{ij} = a_{ji}$
- multiplication: Let  $\mathbf{A} \in R^{m \times s}$ ,  $\mathbf{B} \in R^{s \times n}$

$$AB = C, C \in R^{m \times n}$$

where

$$c_{ij} = \sum_{k=1}^{s} a_{ik} b_{jk}$$

or 
$$c_{ij} = \tilde{\boldsymbol{a}}_i^T \boldsymbol{b}_j$$

- A(BC) = (AB)C
- $AB \neq BA$
- $(AB)^T = B^T A^T$
- I identity matrix: IA = A or AI = A
- inverse (only applies to square matrix):  $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$

### **Examples**

$$\begin{bmatrix} 2 & 3 \\ 6 & 4 \\ 1 & 1 \end{bmatrix} + \begin{bmatrix} 5 & 2 & 2 \\ 1 & 1 & 2 \end{bmatrix} = ?$$

it is not allowed as the dimensions do not match

$$\begin{bmatrix} 2 & 3 \\ 6 & 4 \\ 1 & 1 \end{bmatrix}^T = \begin{bmatrix} 2 & 6 & 1 \\ 3 & 4 & 1 \end{bmatrix}$$

### **Examples**

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### Example

$$\begin{bmatrix} 2 & 3 \\ 6 & 4 \\ 1 & 1 \end{bmatrix} \times \begin{bmatrix} 5 & 2 & 2 \\ 1 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 2 \times 5 + 3 \times 1 \\ c_{21} & c_{22} \\ c_{31} & c_{32} \end{bmatrix}$$
$$\begin{bmatrix} 2 & 3 \\ 6 & 4 \\ 1 & 1 \end{bmatrix} \times \begin{bmatrix} 5 & 2 & 2 \\ 1 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 13 & 7 & 10 \\ 34 & 16 & 20 \\ 6 & 3 & 4 \end{bmatrix}$$
$$\begin{bmatrix} 5 & 2 & 2 \\ 1 & 1 & 2 \end{bmatrix} \times \begin{bmatrix} 2 & 3 \\ 6 & 4 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 24 & 25 \\ 10 & 9 \end{bmatrix}$$

### Example

The inverse of 
$$\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 0 & 5 \end{bmatrix}$$
 is  $\mathbf{A}^{-1} = \begin{bmatrix} 1/3 & 0 \\ 0 & 1/5 \end{bmatrix}$  as  $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$ 

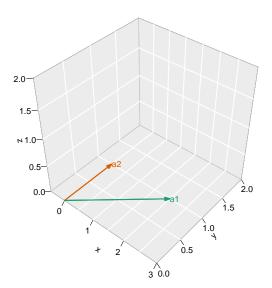
The inverse of I is itself  $I^{-1} = I$ 

### Span, linear independence

- linear combination is just sum of some scaled vectors
  - $\lambda_1 \cdot \boldsymbol{a}_1 + \lambda_2 \cdot \boldsymbol{a}_2 + \ldots + \lambda_n \boldsymbol{a}_n$ ,  $\boldsymbol{a}_i \in R^m$  for  $i = 1, \ldots, n$
  - $a_i$  are vectors (of the same length) and  $\lambda_i$  are the scalars
- span is the set of all possible linear combination

$$\mathsf{Span}(\{\boldsymbol{a}_1,\boldsymbol{a}_2,\ldots,\boldsymbol{a}_n\}) = \left\{\sum_{i=1}^n \lambda_i \boldsymbol{a}_i | \lambda_i \in R, i = 1,\ldots,n\right\}$$

- what is the span of {[1,0]<sup>T</sup>, [0,1]<sup>T</sup>}?
  how about {[2,1]<sup>T</sup>, [0,1]<sup>T</sup>}?
- how about  $\{[2,1]^T, [4,2]^T\}$ ?
- how about  $\{[2,1,0]^T, [0,1,0]^T\}$ ?
  - $\triangleright$  it is a **subspace** (bottom plane) in  $R^3$



• linear independence:  $\{a_1, \ldots, a_n\}$  is linear independent if there exist no  $\lambda_1, \ldots, \lambda_n$  (except all being 0) such that

$$\lambda_1 \cdot \boldsymbol{a}_1 + \lambda_2 \cdot \boldsymbol{a}_2 + \ldots + \lambda_n \boldsymbol{a}_n = \boldsymbol{0}$$

- how about  $\{[2,3]^T, [4,6]^T\}$  ?
- are  $\{[1,0]^T,[0,1]^T\}$  LI?
- essentially a way to tell whether there is any redundant vectors in the set
- rank of a matrix is defined as the maximum number of linearly independent column vectors

### Example

The column vectors of the matrix

$$[\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3] = \begin{bmatrix} 2 & 0 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

are not linearly independent, as

$$\lambda_1 \mathbf{a}_1 + \lambda_2 \mathbf{a}_2 + \lambda_3 \mathbf{a}_3 = \mathbf{0}$$

holds for  $\lambda_1=\lambda_2=1, \lambda_3=-2.$  In other words, one of them is redundant. And rank( $\bf A$ ) = 2

### Matrix vector multiplication

$$\mathbf{A}\mathbf{x} = \begin{bmatrix} | & | & & | \\ \mathbf{a}_1 & \mathbf{a}_2 & \dots & \mathbf{a}_n \\ | & | & & | \end{bmatrix} \begin{vmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{vmatrix} = x_1 \begin{bmatrix} | \\ \mathbf{a}_1 \\ | \end{bmatrix} + x_2 \begin{bmatrix} | \\ \mathbf{a}_2 \\ | \end{bmatrix} + \dots + x_n \begin{bmatrix} | \\ \mathbf{a}_n \\ | \end{bmatrix}$$

- another view of the multiplication
- linear combination of the column vectors of A
  - $x_1 \cdot a_1 + x_2 \cdot a_2 + \ldots + x_n a_n$
  - **a**<sub>i</sub> are the column vectors and x are the scalars
- so . . .  $\mathbf{A}\mathbf{x} = \mathbf{y}$  essentially solves for what ?

### Matrix vector multiplication

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  - a<sub>i</sub> are the column vectors and x are the scalars
- so ... Ax = y essentially solves for what ?
  - y is in the column space of A or not ...
  - if not, then there is no solution
  - if yes, there will be some solution(s)? unique solution or?

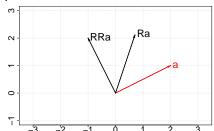
# Matrix vector multiplication (some interpretations)

So  $\boldsymbol{A}\boldsymbol{x}$  is a linear transformation:  $\boldsymbol{x} \to \boldsymbol{y}$ 

ullet Rotation: rotate  ${m x}$  anti-clockwise by  ${m heta}$ 

$$R\mathbf{x} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0.71 & -0.71 \\ 0.71 & 0.71 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

say  $\theta = \pi/4$ 



- $\mathbf{R}$  is a rotation or orthogonal matrix if  $\mathbf{R}^T = \mathbf{R}^{-1}$  (what does it imply?)
  - $\mathbf{R}^T \mathbf{R} = \mathbf{R} \mathbf{R}^T = \mathbf{I}$

reserves length  $(Rx)^T(Rx) = x^T R^T Rx = x^T x$ 

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reserves length  $(\mathbf{R}\mathbf{x})^T(\mathbf{R}\mathbf{x}) = \mathbf{x}^T \mathbf{R}^T \mathbf{R}\mathbf{x} = \mathbf{x}^T \mathbf{x}$ 

Projection (an example): project x to a

$$P(x, a) = ||x|| \cos \theta * \frac{a}{||a||} = \frac{a^T x}{a^T a} a$$
$$= \frac{a \cdot a^T x}{a^T a} = \frac{a a^T}{a^T a} x$$

- $P = \frac{aa^T}{a^Ta}$  is a projection matrix (what is the shape of P?);
- it transforms x to its projection
- what if we project it again (and again and again ...) ? i.e. P(Px)
  - it remains unchanged, PPx = Px

or 
$$PP = P$$

$$\frac{aa^{T}}{a^{T}a} \frac{aa^{T}}{a^{T}a} = \frac{aa^{T}aa^{T}}{(a^{T}a)^{2}} = \frac{aa^{T}}{a^{T}}$$

mathematics is the subject of making sense :-)

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  - or PP = P  $\frac{aa^T}{a^Ta} \frac{aa^T}{a^Ta} = \frac{aa^Taa^T}{(a^Ta)^2} = \frac{aa^T}{a^Ta}$
  - mathematics is the subject of making sense :-)

# Probability theory

- Random variable
- Probability distribution
- Probability mass function and density function
- Probability rules
- Expectation, variance, covariance
- Conditional expectation

### Random variable and probability distribution

# Random variable X associates with a probability distribution P(X)

- formally, a r.v. is a mapping from sample space  $\Omega$  to a target space  ${\mathcal T}$
- e.g. toss a fair coin twice, r.v. X is the number of heads turned up
  - the sample space is  $\Omega = \{HH, TT, HT, TH\}$
  - target space is  $T = \{0, 1, 2\}$
  - · the probability distribution is

$$P(X) = \begin{cases} 0.25 & X = 0 \\ 0.5 & X = 1 \\ 0.25 & X = 2 \end{cases}$$

• the distribution P must satisfy

$$P(X = x) > 0$$
, and  $\sum_{x \in T} P(X = x) = 1$ 

Random variable - discrete r.v.

If r.v. X's target space  $\mathcal{T}$  is discrete

- X is called discrete random variable
- the probability distribution P is called probability mass function (p.m.f.)
- and

$$0 \le P(X = x) \le 1, \text{ and } \sum_{x \in T} P(X = x) = 1$$

### Example - discrete r.v.

**Bernoulli distribution** Tossing a coin, T = H, T,

$$P(X = H) = p, P(X = T) = 1 - p, 0 \le p \le 1$$

**Binomial distribution** Tossing a coin N times, the r.v. X that the number of head shows up is

$$P(X = k) = \binom{N}{k} \cdot p^k (1-p)^{N-k}$$

(convince yourself why)

**Multinoulli distribution** Throw a fair 6-facet die,  $\mathcal{T}=1,2,\ldots,6$ , the distribution is

$$P(X=i)=1/6$$

Verify the above Ps satisfy the requirements of p.m.f.

#### Random variable - continuous r.v.

If r.v. X's target space  $\mathcal T$  is continuous

- X is called **continuous random variable**
- the probability distribution p is called probability density function (p.d.f.)
- and satisfies

$$p(x) \ge 0$$
, and  $\int_{x \in T} p(x) dx = 1$ 

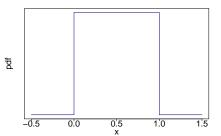
- pdf is not probability as p(x) can be greater 1;
- for  $\forall x \ P(X=x)=0$
- calculate probability over an interval: e.g.

$$P(X \in [a,b]) = \int_a^b p(x) dx$$

### Example - continuous r.v.

**Uniform distribution**  $\mathcal{T} = [0,1]$ , X has equal chance to take any value between 0 and 1; the pdf is

$$p(x) = \begin{cases} 1 & x \in [0, 1] \\ 0 & \text{otherwise} \end{cases}$$



Easy to verify  $\int_0^1 p(x)dx = \int_0^1 dx = 1$ 

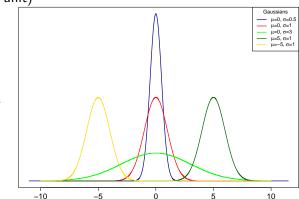
What's the probability that 0 < X < 0.5?

### Example - continuous r.v.

**Gaussian distribution** T = R, or  $X \in R$  the pdf is

$$p(x) = \mathcal{N}\left(x; \mu, \sigma^2\right) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

 $(\frac{x-\mu}{\sigma})^2$  is a distance measure: how far x is away from  $\mu$  (measured by  $\sigma$  as a unit)



Machine Learning, University of St Andrews, Spring 2021

Probability theory, 31/39

### Question

Calculate quickly:

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2} dx = ?$$

For  $X \sim \mathcal{N}(\mu, \sigma)$ , what is  $P(X < \mu) = ?$ 

### Joint distribution

- r.v.  $\boldsymbol{X} = [X_1, X_2, \dots, X_n]^T$  can be multidimensional (each  $X_i$  is r.v.)
  - essentially a random vector
- Still satisfies the same requirements

$$\forall \mathbf{x}, 0 < P(\mathbf{X} = \mathbf{x}) < 1, \ \sum_{x_1} \sum_{x_2} \dots \sum_{x_n} P(\mathbf{X} = [x_1, x_2, \dots, x_n]) = 1$$

or

$$\forall \boldsymbol{x}, p(\boldsymbol{X} = \boldsymbol{x}) > 0, \int \int \dots \int p(\boldsymbol{X} = \boldsymbol{x}) dx_1 dx_2 \dots dx_n = 1$$

• for bivariate case, i.e. n = 2,  $X_1, X_2$  are **independent** if  $P(\mathbf{X}) = P(X_1)P(X_2)$  (e.g. rolling two dice independently)

### Example: discrete joint distribution

The joint distribution of X snow or not,  $Y \in \{\text{spring, summer, autumn, winter}\}$  represents the season that x belongs to :

	y = Spring	y = Summer	y = Autumn	y = winter
x = F	0.05	0.25	0.075	0
x = T	0.2	0	0.175	0.25

It is easy to verify that

$$\sum_{x}\sum_{y}p(x,y)=1$$

### Example: continuous joint distribution

If X, Y's joint p.d.f is

$$p(x,y) = \frac{1}{2\pi\sigma_x\sigma_y}e^{-\frac{1}{2}\left[\left(\frac{x-\mu_x}{\sigma_x}\right)^2 + \left(\frac{y-\mu_y}{\sigma_y}\right)^2\right]}$$

X, Y are bivariate Gaussian distributed (X,Y are independent).

# Probability rules

There are only two probability rules (use integration instead of sum for continuous r.v.):

1. Product rule:

$$p(x,y) = p(y|x)p(x) = p(x|y)p(y)$$

2. Sum rule (marginalisation):

$$p(x) = \sum_{y} p(x, y), \ p(y) = \sum_{x} p(x, y)$$

# Conditional probability

Conditional probability (distribution) by product rule:

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

ullet probability distribution of x conditional on the value of y

	y = Spring	y = Summer	y = Autumn	y = winter
x = F	0.05	0.25	0.075	0
x = T	0.2	0	0.175	0.25

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$$P(Y = \text{Spring})$$
 ? use sum rule  $P(Y = \text{Spring}) = \sum_{X=\{T,F\}} P(X = T, Y = \text{Spring}) = 0.05 + 0.2 = 0.25$ 

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$$P(X = T | Y = Spring)$$
 ?  
 $P(x = T | y = Spring) = \frac{P(x = T, y = Spring)}{P(y = Spring)} = \frac{0.05}{0.25} = 0.2$ 

### Expectation and variance

**Expection** of a r.v. is defined as

$$E[X] = \sum_{x} xP(x) \text{ or } E[X] = \int xP(x)dx$$

Variance of a r.v. is defined as

$$var[X] = \sum_{x} xP(x) \text{ or } E[X] = \int xP(x)dx$$

### Reference