

Computational Geoscience

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Who, what, where?

- The course team:
 - Andrew Valentine
 - Rebecca McGirr
- For the next three weeks:
 - Mon/Wed/Thur/Fri: 10-12
 - Wed/Fri: 2-5
- All classes will be online via Zoom
- Classes will be focused on practical exercises

Assessment

- In-class assessment (20%)
 - 10-12 Thurs 7th May
 - Please see me today if there is any chance you cannot attend for this
- Assessed programming project
 - More details towards the end of the course
 - Due: 5pm Friday 5th June
- Four optional drop-in sessions will be held:
 - Dates/times tbc...
 - Opportunity to ask questions and get help
 - No need to attend if you have no questions!

Assessment

- Assessed programming project
 - More details towards the end of the course
 - Due: 5pm Friday 5th June
- When you get stuck, you are encouraged to:
 - Talk to friends/colleagues
 - Make use of online resources
- However, you must
 - Write your code yourself: don't copy and paste from a friend's solution or a website
 - Understand how your solution works
 - Be able to explain why you chose to solve the problem the way you did

Assessment

- Assessed programming project
 - More details towards the end of the course
 - Due: 5pm Friday 5th June
- Graded based on:
 - Submitted solution to the task, and
 - Oral examination (via Zoom; 15-20 minutes)
- If you do not attend the oral examination you will receive no credit!
- Oral examinations will be arranged for the week commencing 8th June (dates and times to be confirmed). If you expect to be unavailable during this week please talk to me today.

Please give us feedback...!

- If you have any comments or suggestions about the course (or its online delivery), please get in touch!
 - Talk to/email me or Rebecca
 - Send a message via the AD Honours/Masters (Dr Rhodri Davies)
 - SELT? Not running during COVID-19?

"I think it would be worthwhile to mention in the first lecture that learning programming can be a **steep learning curve** for some people and that **it does get easier** the more you use it and once you are able to debug code. Initially, I was doubtful at my ability to learn python and do well in the course which temporarily decreased my productivity and motivation to succeed."

Student, 2019

Why?

Why does a geoscientist need to know about programming?

What is a programming language?

What is an algorithm?



How do you make a cup of coffee?

- Need to spell everything out carefully no shortcuts or assumptions
- Task can be broken into sub-tasks, e.g.
 "boil kettle", provided they are well-defined
 - Sub-task may appear in other contexts,
 e.g. to make tea or hot chocolate







How do you make dinner?

- Our 'recipe' for coffee works with any mug
- 'Mug' in the recipe is an abstract object assumed to have certain properties





Can you make coffee in a bucket?

Can you make coffee in a cat?



A *type definition* is a set of rules defining the properties and behaviours we can expect a certain object to have.

Every object is an *instance* of some abstract type. It is guaranteed to have all the properties and behaviours set out in the type definition.

- Our 'recipe' for coffee works with any mug
- 'Mug' in the recipe is an abstract object assumed to have certain properties
- When we execute the recipe, we select a real, physical mug and let it 'stand in for' the abstract entity



A function or subroutine is a sequence of instructions designed to perform a particular task, packaged into readily-reusable form.

- To use a function, we only need to understand its interface – we don't care about how it works internally
 - What information do we have to give to the function? ('Arguments')
 - What information does it give us back? ('Return value')



Programming is like Lego - we connect lots of simple pieces together to make something much more sophisticated

$$1+2+3+...+10 = ?$$

Recap

- To tackle a complex problem, we break it down into manageable pieces.
- First understand the **algorithm** we want to create, then worry about how to **implement** that in a particular **programming language**.
- Important to spell everything out in detail computers are dumb.
- Write generic 'recipes' or functions that work for all objects of a certain type
- Then call the function passing it specific instances as arguments

I am thinking of a number between 1 and 10...

A variable is a named 'slot' in which a piece of information can be stored temporarily, accessed and updated.

A variable has an associated type.

A *constant* is a piece of information which is built into a program and cannot be changed.

Variables and constants are stored in your computer's RAM (random access memory)

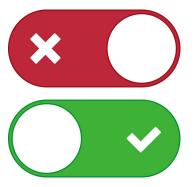
Computing is built around the binary system

- Information is stored using bits (binary digits)
- A bit can take the value 0 or 1 it's essentially a switch
- To represent more complex information we combine bits

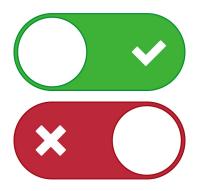


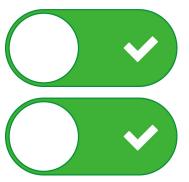


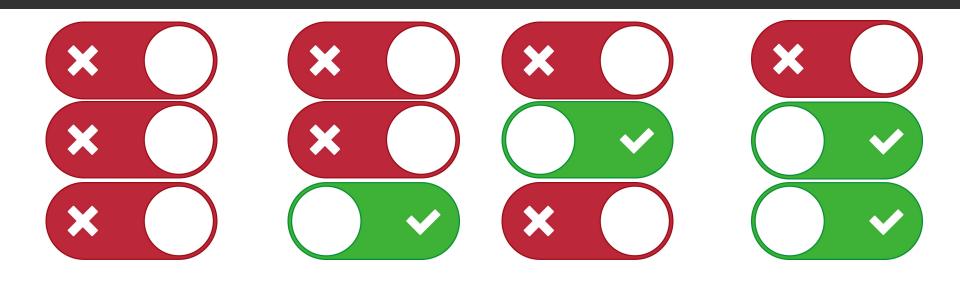




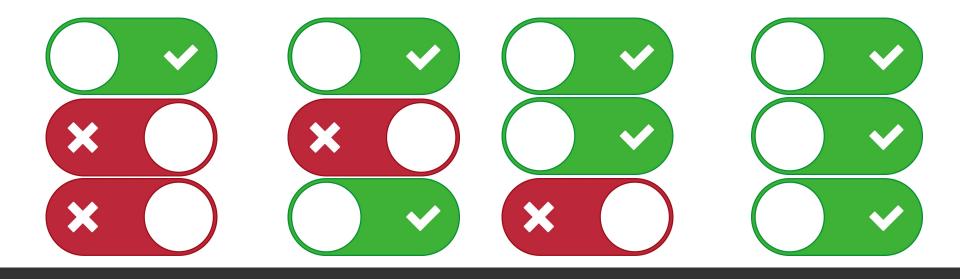
A 2-bit system has 4 states







A 3-bit system has 8 states



In general, a set of N bits can represent 2^N different states

- We can only represent a finite, discrete (countable) set of quantities
- Every kind of information must be mapped onto this discrete set

N	2 ^N
1	2
2	4
3	8
4	16
5	32
6	64
7	128
8	256
16	65536
32	4294967296
64	$\approx 1.845 \times 10^{19}$

A byte is a unit of 8 bits

A *kilobyte* is 2¹⁰=1024 bytes A *megabyte* is 2²⁰ bytes (1024 kilobytes) A *gigabyte* is 2³⁰ bytes (1024 megabytes) And so on: terabytes, petabytes, exabytes...

NB: Sometimes kilo-/mega-/giga- etc are used in their usual SI sense, i.e. $10^3/10^6/10^9$ bytes. An SI terabyte is only 90% the size of a base-2 terabyte!

Three main 'building blocks' of information:

- Integers (1,2,3,...)
- Real/floating-point numbers (1.326, -2.33162, π,...)
- Alphanumeric characters ('a', 'b', '1',...

Integers are already discrete, so can easily be mapped onto binary system

- 1. Choose how many bits you are going to use (typically 32 bits/4 bytes)
- 2. Decide whether you need to represent negative numbers
- 3. Decide whether to read the bits from left-to-right or right-to-left ('big endian or little endian')

	$0 0 0 \rightarrow 0$	$0 0 0 \rightarrow 0$	
Unsigned	$0.01 \rightarrow 1$	$001 \rightarrow 1$	
	$010 \rightarrow 2$	$010 \rightarrow 2$	
	$011 \rightarrow 3$	$011 \rightarrow 3$	
	$1 0 0 \rightarrow 4$	$100 \rightarrow ?$	Signed
	$101 \rightarrow 5$	1 0 1 → -1	
	$110 \rightarrow 6$	$1\ 1\ 0 \rightarrow -2$	
	$111 \rightarrow 7$	1 1 1 → -3	

Alphanumeric data is also discrete and easy to map, by defining a standard ordering:

```
000 \rightarrow a
001 \rightarrow b
010 \rightarrow c
011 \rightarrow d
100 \rightarrow A
101 \rightarrow B
110 \rightarrow C
111 \rightarrow D
```

Usually the ASCII (American Standard Code for Information Interchange) table is used...

Decimal	Hexadecimal	Binary	0ctal	Char	Decimal	Hexadecimal	Binary	0ctal	Char	Decimal	Hexadecimal	Binary	0ctal	Char
0	0	0	0	[NULL]	48	30	110000	60	0	96	60	1100000	140	*
1	1	1	1	[START OF HEADING]	49	31	110001	61	1	97	61	1100001	141	a
2	2	10	2	[START OF TEXT]	50	32	110010	62	2	98	62	1100010	142	b
3	3	11	3	[END OF TEXT]	51	33	110011	63	3	99	63	1100011	143	C
4	4	100	4	[END OF TRANSMISSION]	52	34	110100	64	4	100	64	1100100	144	d
5	5	101	5	[ENQUIRY]	53	35	110101	65	5	101	65	1100101	145	е
6	6	110	6	[ACKNOWLEDGE]	54	36	110110		6	102	66	1100110		f
7	7	111	7	[BELL]	55	37	110111		7	103	67	1100111		g
8	8	1000	10	[BACKSPACE]	56	38	111000		8	104	68	1101000		h
9	9	1001	11	[HORIZONTAL TAB]	57	39	111001		9	105	69	1101001		i
10	A	1010	12	[LINE FEED]	58	3A	111010		:	106	6A	1101010		i
11	В	1011	13	[VERTICAL TAB]	59	3B	111011		;	107	6B	1101011		k
12	С	1100	14	[FORM FEED]	60	3C	111100		<	108	6C	1101100		1
13	D	1101	15	[CARRIAGE RETURN]	61	3D	111101		=	109	6D	1101101		m
14	E	1110	16	[SHIFT OUT]	62	3E	111110		>	110	6E	1101110		n
15	F	1111	17	[SHIFT IN]	63	3F	111111		?	111	6F	1101111		0
16	10	10000	20	[DATA LINK ESCAPE]	64	40	1000000		@	112	70	1110000		р
17	11	10001	21	[DEVICE CONTROL 1]	65	41	1000001		Ä	113	71	1110001		q
18	12	10010	22	[DEVICE CONTROL 2]	66	42	1000010		В	114	72	1110010		r
19	13	10011	23	[DEVICE CONTROL 3]	67	43	1000011		C	115	73	1110011		s
20	14	10100	24	[DEVICE CONTROL 4]	68	44	1000100		D	116	74	1110100		t
21	15	10101	25	[NEGATIVE ACKNOWLEDGE]	69	45	1000101		E	117	75	1110101		u
22	16	10110	26	[SYNCHRONOUS IDLE]	70	46	1000110		F	118	76	1110110		v
23	17	10111	27	[ENG OF TRANS. BLOCK]	71	47	1000111		G	119	77	1110111		w
24	18	11000	30	[CANCEL]	72	48	1001000		H	120	78	1111000		x
25	19	11001	31	[END OF MEDIUM]	73	49	1001001		ï	121	79	1111001		y
26	1A	11010	32	[SUBSTITUTE]	74	4A	1001010		j .	122	7A	1111010		z
27	1B	11011	33	[ESCAPE]	75	4B	1001011		ĸ	123	7B	1111011		{
28	1C	11100	34	[FILE SEPARATOR]	76	4C	1001100		Ĺ	124	7C	1111100		ì
29	1D	11101	35	[GROUP SEPARATOR]	77	4D	1001101		М	125	7D	1111101		}
30	1E	11110	36	[RECORD SEPARATOR]	78	4E	1001110		N	126	7E	1111110		~
31	1F	11111		[UNIT SEPARATOR]	79	4F	1001111		0	127	7F	1111111		[DEL]
32	20	100000		[SPACE]	80	50	1010000		P					
33	21	100001		1	81	51	1010001		Q					
34	22	100010			82	52	1010010		R					
35	23	100011		#	83	53	1010011		S					
36	24	100100		\$	84	54	1010100		Т					
37	25	100101		%	85	55	1010101		Ü					
38	26	100110		&	86	56	1010110		V					
39	27	100111		F.	87	57	1010111		w					
40	28	101000		(88	58	1011000		X					
41	29	101001		j	89	59	1011001		Ŷ					
42	2A	101010		*	90	5A	1011010		Z					
43	2B	101011		+	91	5B	1011011		ī					
44	2C	101100		,	92	5C	1011100		Ň					
45	2D	101101			93	5D	1011101		ì					
46	2E	101110			94	5E	1011110		^					
47	2F	101111		i	95	5F	1011111							
				-					-	'				

Real numbers are harder: we have to discretize them

- Cannot represent most numbers exactly
- Common source of 'numerical error' in calculations

Represent a.bcde as p x 2q where p and q are integers

Floating point arithmetic can give weird results...

Any number 'too large' to be representable is assumed to be infinity

Any number 'too small' to be representable is assumed to be 0

You will sometimes see values of 'NaN', meaning 'Not A Number' – this means something weird happened in your calculation