# Species distribution models (SDM) – from a computer perspective

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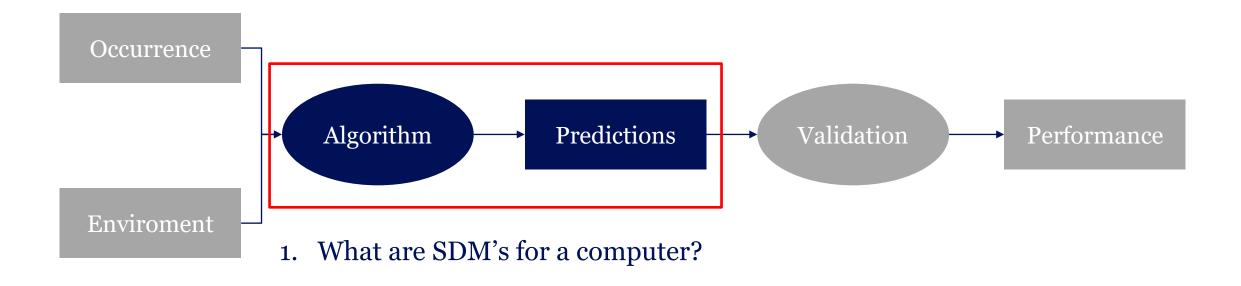
Systematics & Biodiversity, 2020







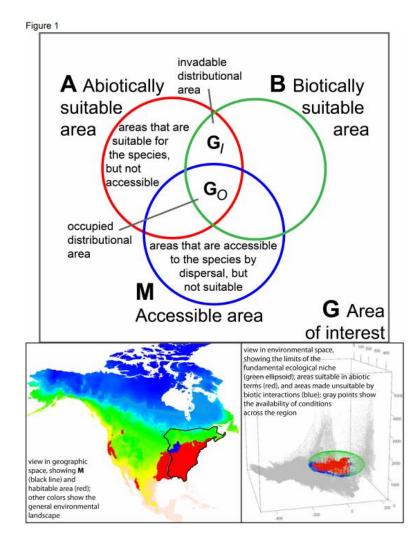
#### Remember where we are:



- 2. How does it understand the niche?
- 3. How does it predict?

- Defining Ecological Niches: Hutchinson
  - n-dimensional **Environmental** space ("hyperspace")
  - **Sóberon & Peterson**: Abiotic, Biotic, Movement
  - Geographic space (where they are) vs Niche space (why they are there)
- From a more formal point of view:

EN(species) = f(Abiotic, Biotic, Movement)

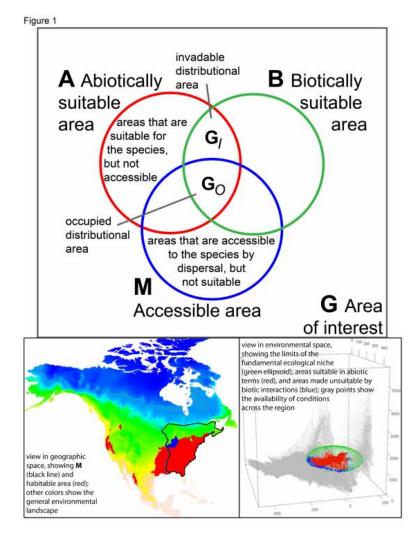


From: https://doi.org/10.1515/eje-2015-0014

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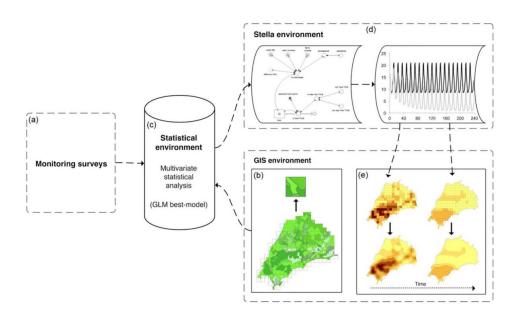
- But.. There is no "Ecological niche value" (EN)
  - And also, no "f(A,B,M)"
- Two **competing approaches**:
  - Probabilistic models "vs" Mechanistic models



From: https://doi.org/10.1515/eje-2015-0014

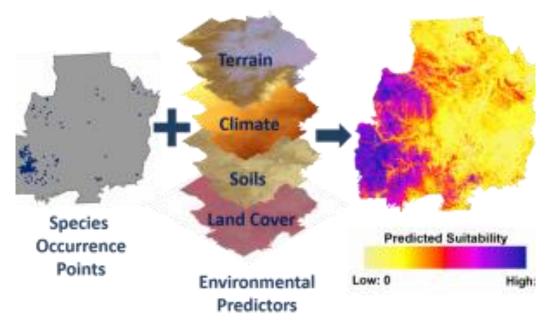
• Two "competing" approaches: Focus will be on Probabilistic models

#### Mechanistic models



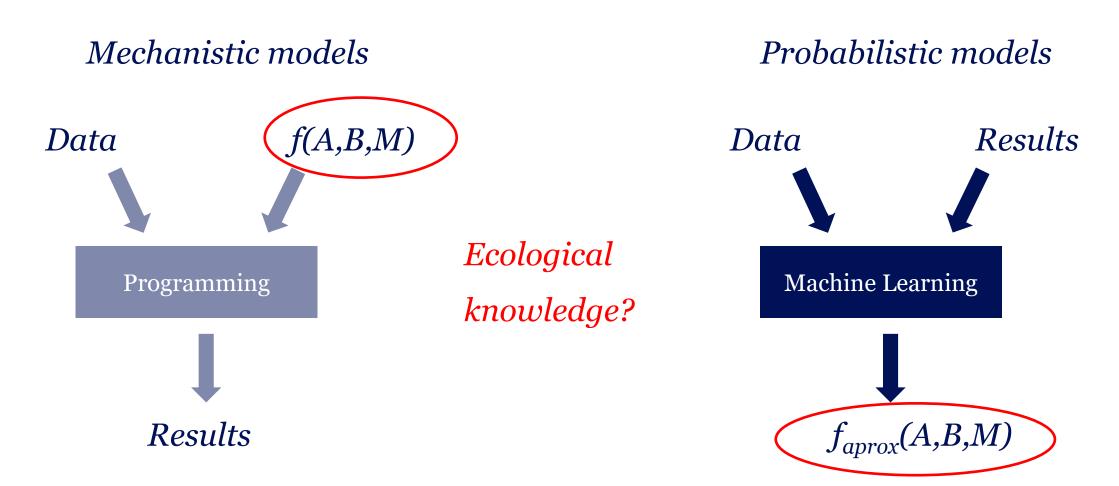
From: https://doi.org/10.1016/j.biocon.2017.04.013

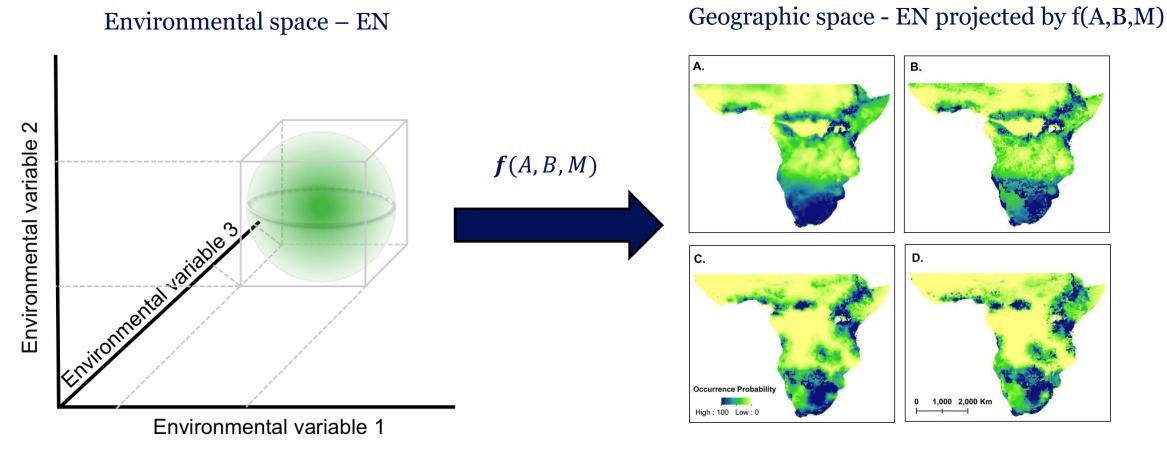
#### Probabilistic models



From: <a href="https://www.natureserve.org/conservation-tools/habitat-suitability-modeling">https://www.natureserve.org/conservation-tools/habitat-suitability-modeling</a>

Two "competing" approaches: Focus will be on Probabilistic models



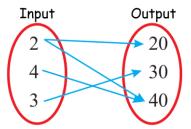


From: https://doi.org/10.4404/hystrix-27.1-11678

If the EN was a simple n-dimentional surface... It would be easy....

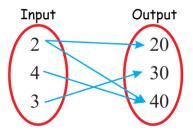
- Machine learning:
  - At the core: learning a mapping function
  - Mapping function: "arbitrary" function Translates/transforms input values from one domain to another

F(input) = Output



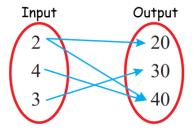
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- AKA: Ecological niche models; Habitat/Suitability modelling; Correlative models, Range mapping; etc
  - For ML people: Supervised learning
  - Commonly maps: N-dimensions onto 1D probability
  - PS: More common problem in supervised learning is to map N:M dimensions

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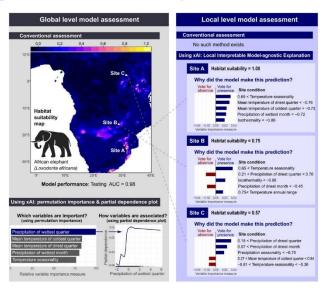


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  - Commonly maps: N-dimensions onto 1D probability
  - PS: More common problem in supervised learning is to map N:M dimensions
- Risks: (<u>Timnit Gebru</u>)
  - Bad data -> bad model
  - Biases in data -> biases in the model
  - "black-box" (or maybe not... Increasingly debatable!)

F(input) = Output



Explainable AI is arriving! (PS: R code available!)



From: <a href="https://doi.org/10.1111/ecog.05360">https://doi.org/10.1111/ecog.05360</a>

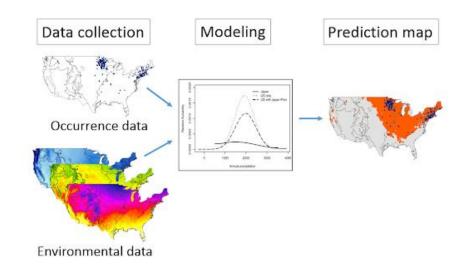
- Having occurrence data and environmental data
  - we want to find the P(Species) being present given the environment
- Formalizing from a Bayesian perspective:

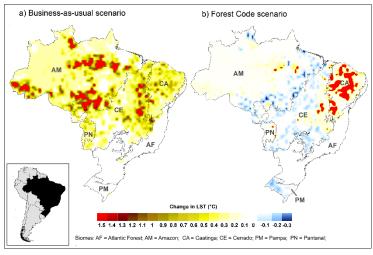
$$P(Species|Env) = \frac{P(Env|Species) \cdot P(Species)}{P(Env)}$$

• Implies that: P(Species), P(Env) are independent

But, are they?

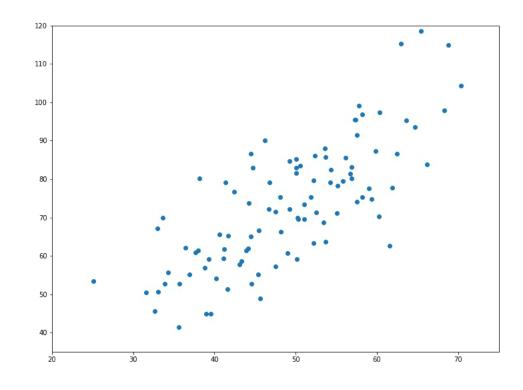
 Objective: learn a function that maps environmental variables onto a 1D probability of occurrence





From: https://doi.org/10.1371/journal.pone.0213368

- How do machines actually, learn?
- Consider you are asked to find the best linear model that fits a set of data
  - And you skipped the linear algebra class
  - But you know that: Y = mX + C is a linear equation
  - And m is the "slope" and C is the "bias"



- How do machines actually, learn?
- Consider you are asked to find the best linear model that fits a set of data
  - And you skipped the linear algebra class
  - But you know that: Y = mX + C is a linear equation
  - And m is the "slope" and C is the "bias"
- A smart solution would be to draw a line that "more or less fits" the data
  - Solve the system for m and C:  $\begin{cases} Y_{\chi} = mX + C \\ Y_{0} = C \end{cases}$

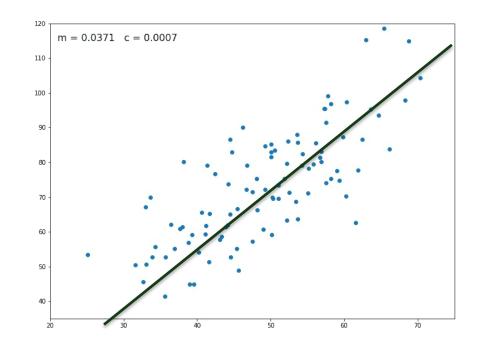


You'll only sucessfully "cheat" if you <u>choose a</u> good enough linear model.. AKA trial and error

- Machine's learn by "trial & error".
  - Computers excel at quickly trying everything
- They find the best parameters so that:
  - Some measurement of error is minimized
  - E.g:  $|| Y(parameters) E(Y) || \approx O$
  - This is often called the "objective/cost/loss":

$$Cost(m,C) = |Y_{(m,C)} - E(Y)|$$

- Finding the best set of parameters <u>becomes an</u> <u>optimization problem</u>
  - As in, finding the optimal solution to a problem



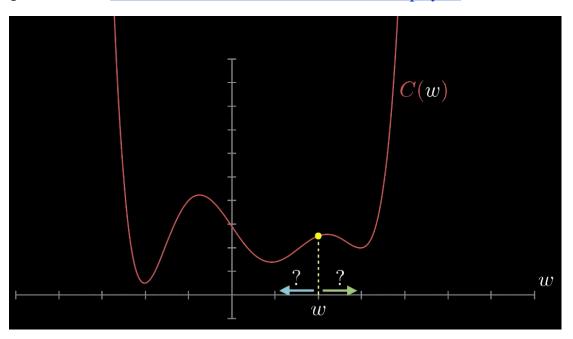
Good choice!

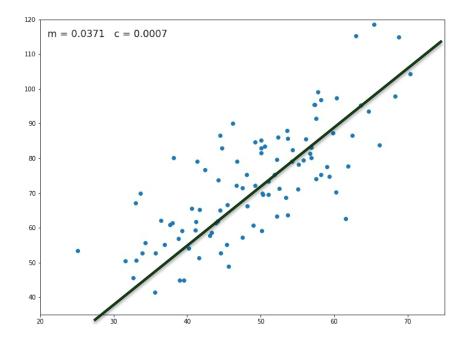
The model "unit"

$$Y = m X + C$$

$$\downarrow$$
Parameters

3blue1brown: "But what is a neural network?" - Youtube playlist





- If we would just try different random sets of parameters we might never find the best solution
- So computers generally <u>start random but then in each iteration focus on the sets</u> <u>that have the best results</u>

What we hope in the end is:

P(Species | Env): Learn a function: Geographical space f(A, B, M) = P(species)

From: <a href="https://doi.org/10.1111/ivb.12113">https://doi.org/10.1111/ivb.12113</a>

# Any questions? 30s



#### Bioclimatic envelope

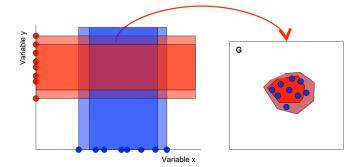
- Find best "rule" (aka threshods) that groups the data into similar sets
- AKA: minimizing the impurity

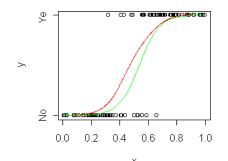
#### Generalized Linear model (Logistic)

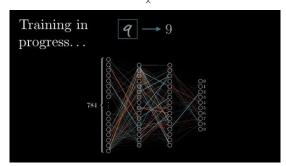
 Finds the best parameters in a linear model structure that minimizes the ||Y - Y\_expected||

#### Artificial neural networks

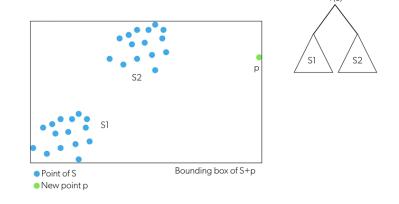
- Sets of directed input/output linear models compressed into nonlinear functions
- Minimizes the difference between the ||Y Y\_expected||



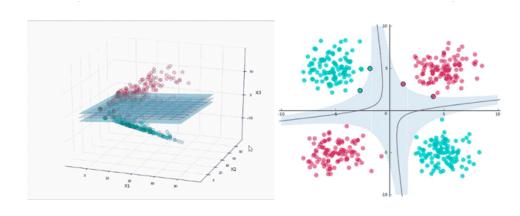




- Random forests and Decision tree's
  - Creates a hierarchy of rules that bins similar groups into the same by minimizing their impurity
  - Final output is a weighted sum of regression models on each bin



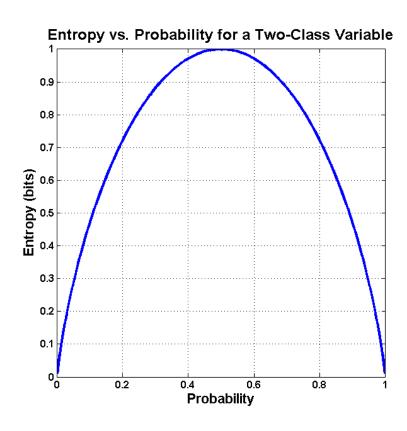
- Support vector machine
  - Projects data into another space
  - Find the best n-dimensional plane that separates the data on the new space AKA maximizes separability
- There are dozens/hundreds of algorithms, but our focus will in MAXENT



- MAXENT
  - <u>Maximum entropy principle</u>
  - AKA the best model is the one that is constrained by the data but has the highest uncertainty
  - One of the benefits of MAXENT SDM is that they only needs presence points
- Entropy can be defined as measure of disorder or uncertainty
- If a coin toss is unbiased, each side has 50% probability



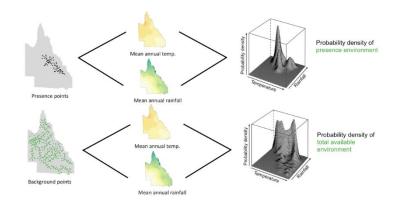
- The entropy is maximized -> you are the most uncertain about the outcome
- If the coin has a bias -> less entropy
- Applying the Maximum entropy principle:
  - For any possible probability distribution, choose the most uncertain possible
  - OR: Maximize a measure of uncertainty



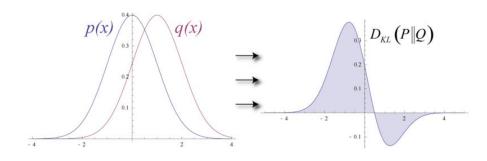
- The most uncertain case for a species distribution:
  - A P(Species|Env) where it species is equally likely to occur in every location
  - In MAXENT: Background distribution
- Imposes the structure of a <u>Gibbs</u> distribution to the environment:

$$P(X=x)=rac{1}{Z(eta)}\exp(-eta E(x)).$$

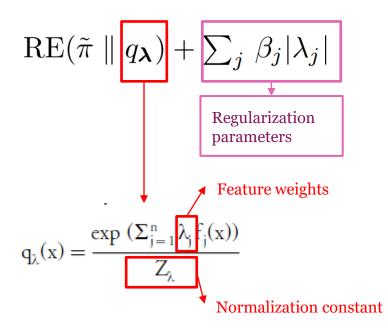
- MAXENT in machine learning:
  - Minimizes the difference between the observed distribution (presences) and the random background distribution (generated pseudo-absences)
  - Uses the <u>relative entropy</u> formula to measure their difference

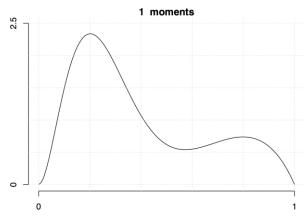


From: <a href="https://onlinelibrary.wiley.com/doi/full/10.1111/j.1472-4642.2010.00725.">https://onlinelibrary.wiley.com/doi/full/10.1111/j.1472-4642.2010.00725.</a>



- How does the <u>model maths</u> look like?
  - Deeply discussed in Phillips, 2004
  - RE is the relative entropy operator symbol
  - $\pi$ -tilde is the observed probability distribution
  - $q_{\lambda}$  is the background distribution parametrized by the <u>Gibbs</u> measure (<u>also</u>)
  - $\beta_i |\lambda_i|$  -> are regularization parameters to curb over fitting.
- Notice, it changes only the parameters of the background distribution  $(q_{\lambda})$  and not the presence distribution
- In SDM terms, MAXENT aims to:
  - Find the most uncertain distribution that is constrained by the observed presence points
  - Os, in other words: Starts with the most random distribution possible and finds the most random distribution possible that still predicts the presences

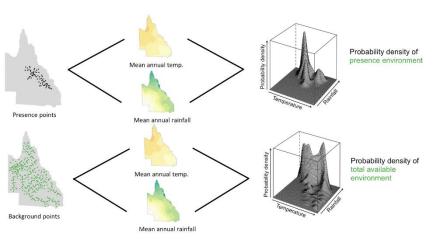




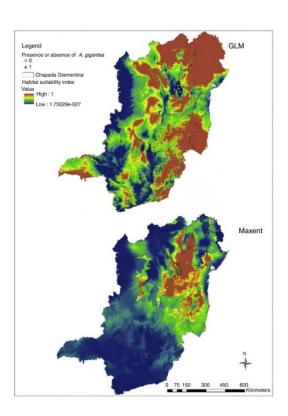
Mine both probability distributions from the data and learn the parameters

Apply the bayes theorem!

And voilá



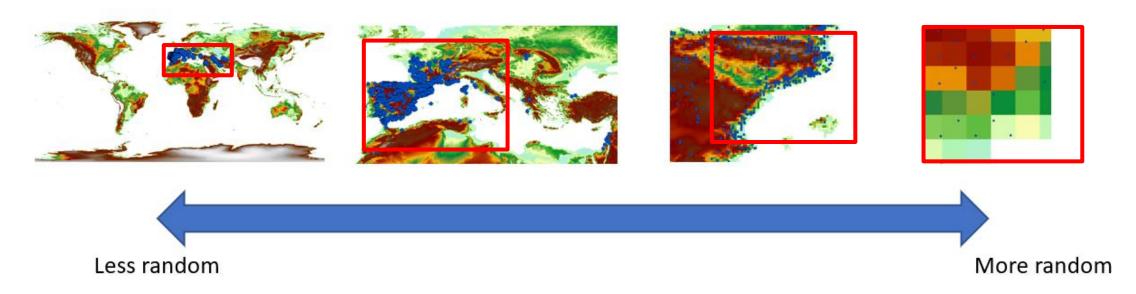
$$P(S|E) = \frac{P(S|E) \cdot P(S)}{P(E)}$$



From: https://onlinelibrary.wiley.com/doi/full/10.1111/j.1472-4642.2010.00725.x

From: https://doi.org/10.1016/j.ncon.2015.03.001

- SDM can be limited by:
  - Environmental space not being representative of the process -> Problem of scale



- The processes defining the distribution of the species vary according to the scale that you are using!
  - Machine learning, with bad data in will just produce a bad model -> it will learn how to do random predictions.

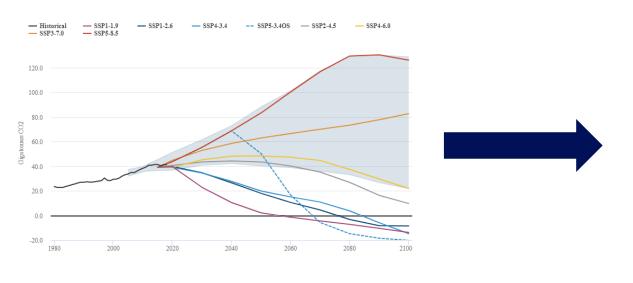
- SDM can be limited by:
  - Spatial biases



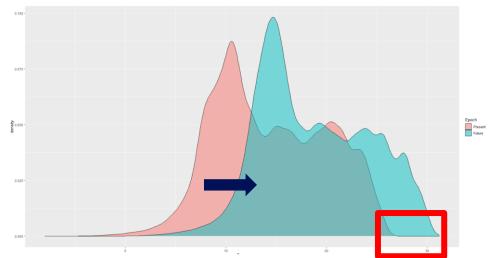


- Different sampling designs are also part of the processes that Machine learning learns
  - Meaning, if your data sampling strategy is biased, your model, will also learn that bias

- SDM can be limited by:
  - Non-analogous conditions in time

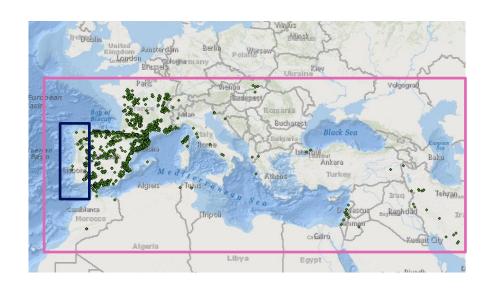


Present vs 50 years in the future (rocky road scenario!)

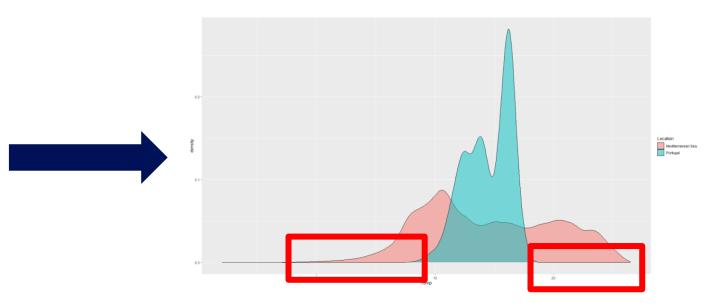


- Above we see a shift both in the distribution (arrow) as well as a range of values outside the training range(red box) for the Mean Annual temperature in the study area
- These non-analogous conditions imply that your model is extrapolating on that range

- SDM can be limited by:
  - Non-analogous conditions in space



Temperature distribution for Portugal and the Mediterranean



- A model trained in Portugal would have to extrapolate if used in the Mediterranean regions.
- Mismatch is an environmental space problem occurs frequently with Invasive Alien Species

- So in summary:
  - All ML models have a set of parameters and structure which is optimized to fit observations
  - Machine learning is able to "understand" the processes but can't (necessarely) explain them to humans
- The ML behaviour is fully driven by:
  - Model structure
  - Parameter
  - Cost function and optimization method
- At the end of the procedure you have a function (f) that:
  - maps an n-hyperdimensional space onto another n-hyperdimensional space
  - In SDM: **n-Environmental space** to probabilistic space -> which then can be projected to a **Geographical space**

#### • Error sources:

- Spatial biases: are a process that can (will) get learned by the algorithm
- Scale: affects the driving spatial processes defining the distributions -> your model learns what you give it
- Non-analogous conditions in time & space: The model has to extrolate

#### Not all models work the same:

• MAXENT works "fine" even with reduced sample numbers – maximum entropy principle

#### Most important for a good SDM model:

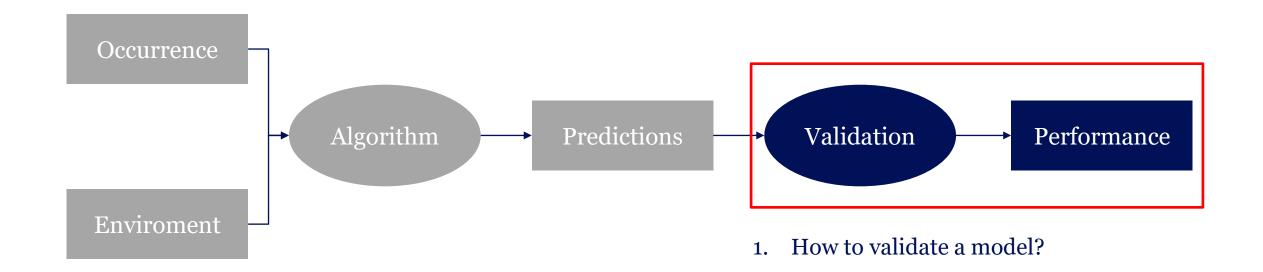
- Occurrence data reflecting the ecological niche of the species
- A scale that reflects the ecological processes that you want to investigate <- one of the big problems
- A model that "maximizes" your objectives: Excellent predictions? Deep Learning

## Any questions? 1min

### Next: Validating your model

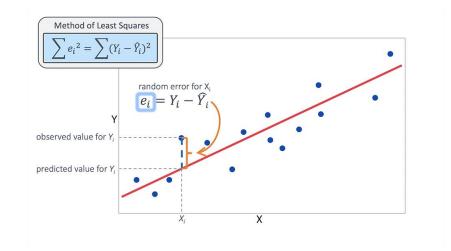


#### Remember where we are:



- 2. How to interpret the relations on the data?
- 3. What are the limitations of the model?

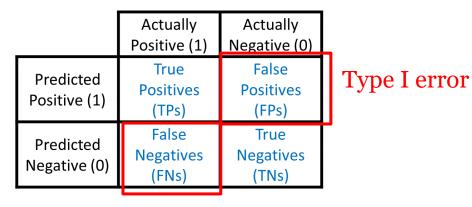
- In ML there are <u>two main types</u> of validations:
  - Regressions errors: Root mean squared error, Mean absolute error etc
  - Classification errors: Overall acuraccy, K, jaccard etc.
- SDM is a <u>supervised classification</u> exercise
  - Binary: the species is either Present or Absent
  - Even if in some cases, the output is a Probability
  - Threfore, use classification validation metrics
- Classification errors:
  - Mostly based on the concept of Confusion matrix (next)



		True condition				
	Total population	Condition positive	Condition negative	$= \frac{\text{Prevalence}}{\sum \text{Total population}}$	Σ True pos	curacy (ACC) = sitive + Σ True negative Total population
Predicted	Predicted condition positive	True positive	False positive, Type I error	Positive predictive value  (PPV), Precision =  Σ True positive Σ Predicted condition positive	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$ Negative predictive value (NPV) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Predicted condition negative}}$	
condition	Predicted condition negative	False negative, Type II error	True negative	$\frac{\text{False omission rate (FOR)} = }{\Sigma \text{ False negative}}$ $\Sigma \text{ Predicted condition negative}$		
		True positive rate (TPR), Recall, Sensitivity, probability of detection, Power = \( \sum_{\text{True positive}} \) \( \sum_{\text{Condition positive}} \)	False positive rate (FPR), Fall-out, probability of false alarm = Σ False positive Σ Condition negative	Positive likelihood ratio (LR+) = TPR FPR	Diagnostic odds ratio	F <sub>1</sub> score =
		False negative rate (FNR),  Miss rate  = Σ False negative Σ Condition positive	Specificity (SPC), Selectivity, True negative rate (TNR) = Σ True negative Σ Condition negative	Negative likelihood ratio (LR-) = FNR TNR	(DOR) = LR+ LR-	2 · Precision · Recall Precision + Recall

- Confusion matrix: (aka error matrix)
  - Shows the agreement between our predictions and the validation data
- The values represent the times our predictions agreed or disagreed with the validation data
  - Type I error -> our model predicted the species where it is absent
  - Type II error -> our model didn't predict the species where it is present
- Remember, our outputs of MAXENT are probabilities [0 to 1] so:
  - We have to select a minimum probability (e.g. 50%) after which the species is present

#### **Confusion Matrix**



Type II error

		True condition				
	Total population	Condition positive	Condition negative	$= \frac{\text{Prevalence}}{\sum \text{Total population}}$	Σ True pos	curacy (ACC) = sitive + Σ True negative otal population
Predicted	Predicted condition positive	True positive	False positive, Type I error	Positive predictive value  (PPV), Precision =  Σ True positive Σ Predicted condition positive	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$	
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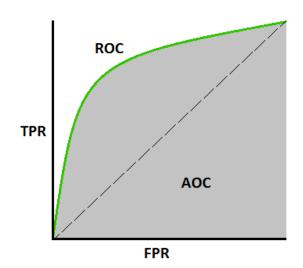
#### Problem!

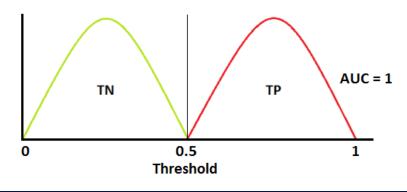
- Absences are especially difficult to define in the context of Species Distribution Models
- MAXENT does not need to use Presence and Absence data
- Without Presence/Absence data we cannot use the confusion matrix

#### • The alternative:

- An estimate of the models ability to discriminate the species from the environment
- This metric is know as <u>Area under the curve of the Receiver operating</u> characteristic (AUC-ROC)

- Receiver operating characteristic curve (ROC)
  - Ilustrates the ability of the binary classifier by varying the probability threshold
  - Notice: both axis vary from 0 to 1
- TPR = Sensitivity
  - Tells something about the ability to predict true positives
- FPR = 1 Specificity
  - Tells something about the ability to identify true negatives
- Area-under the curve (AUC):
  - Integral of the area under the ROC curve.
  - When the discrimination power is perfect: AUC=1

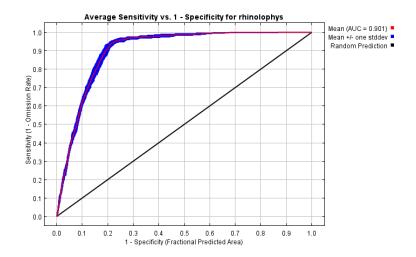




- Problem still remains in MAXENT!
  - No Presences and absences available!
- MAXENT actually uses the Area of the predictions to produce the AUC-ROC:

$$TPR_{maxent} = 1 - A_{FOR} = 1 - \frac{A_{FN}}{A_{FN} + A_{TN}}$$
 $FPR_{maxent} = 1 - A_{PPV} = 1 - \frac{A_{TP}}{A_{TP} + A_{FP}}$ 

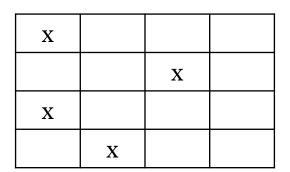
- Where the  $A_{ij}$  represents:
  - The actual geographical area predicted as FN, TN, TP,FP



		True condition					
	Total population	Condition positive	Condition negative	$\frac{\text{Prevalence}}{\sum \text{Condition positive}} = \frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Σ True pos	curacy (ACC) = sitive + Σ True negative Total population	
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		$\label{eq:transformation} \begin{split} & \text{True positive rate (TPR),} \\ & \text{Recall, Sensitivity,} \\ & \text{probability of detection, Power} \\ & = \frac{\Sigma  \text{True positive}}{\Sigma  \text{Condition positive}} \\ & \text{False negative rate (FNR),} \\ & \text{Miss rate} \\ & = \frac{\Sigma  \text{False negative}}{\Sigma  \text{Condition positive}} \end{split}$	False positive rate (FPR), Fall-out, probability of false alarm $= \frac{\sum False positive}{\sum Condition negative}$ Specificity (SPC), Selectivity, True negative rate (TNR) $= \frac{\sum True negative}{\sum Condition negative}$	Positive likelihood ratio (LR+) = TPR FPR  Negative likelihood ratio (LR-) = FNR TNR	Diagnostic odds ratio (DOR) = LR+ LR-	F <sub>1</sub> score = 2 · <u>Precision · Recall</u> Precision + Recall	

"When AUC statistics are applied to presence-only data and pseudo-absences, the maximum achievable AUC value is no longer 1, BUT 1- a/2; where a stands for the true species' distribution, which we typically do not know" (Phillips, 2006)

Less prevalent



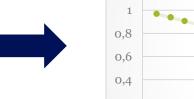
$$1 - \frac{\frac{4}{16}}{2} = 1 - 0.125 = 0.875$$

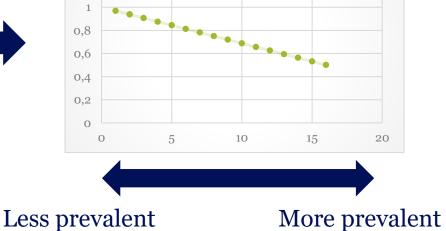
$$1 - \frac{\frac{10}{16}}{2} = 0.6875$$

#### More prevalent

X		X	
	X	X	X
X		X	X
	X	X	

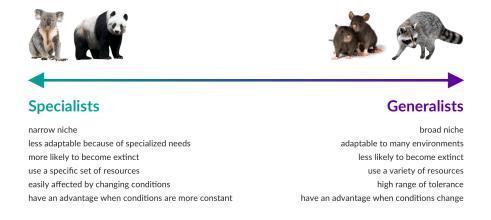
$$1 - \frac{\frac{10}{16}}{2} = 0.6875$$



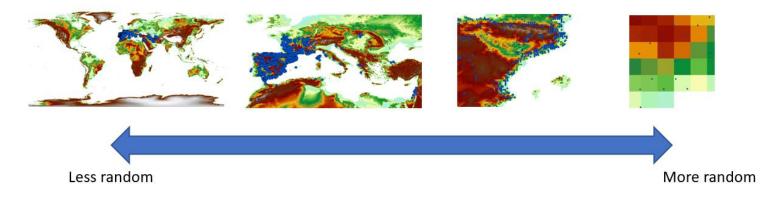


MaxAUC

The implication that the AUC is vulnerable to generalist/specialist species



### And also <u>highly sensitive to the Scale:</u>

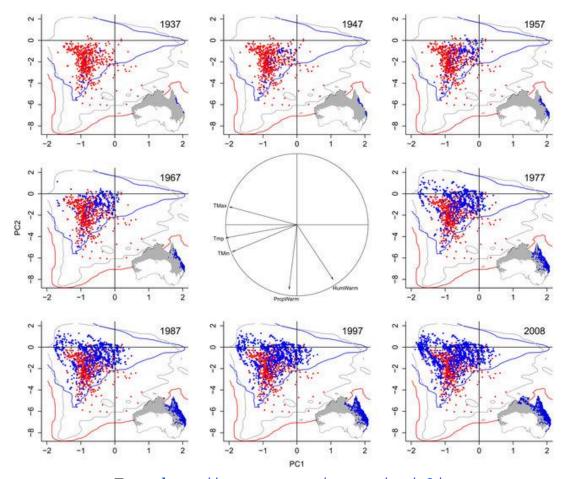


- In summary:
  - SDM can and should be validated using regular classification error metrics
  - MAXENT is a special case where absence data is "not available"
- MAXENT is usually validated using the AUC-ROC curve
  - Software provides it! So don't worry
- AUC is highly affected by prevalence & scale
  - MAXENT goes around it by considering background data as pseudo-absence
- There are other methods to validate! Of course!
  - E.g. a Leiden research proposed a Null-model approach (Neils Raes, 2007)

# Any questions? 30s



- Non- analogous conditions
  - In time (e.g. Climate change)
  - In space (e.g. A new geographical region)
- There are other methods but not explored today
- We'll focus on the solutions MAXENT offers
  - Model response curves & clamping
  - Multivariate Environmental Similarity Surfaces (MESS) & Most dissimilar variable (MoD)
  - Variable importance & Jacknife testing



From: <a href="https://www.pnas.org/content/111/28/10233">https://www.pnas.org/content/111/28/10233</a>

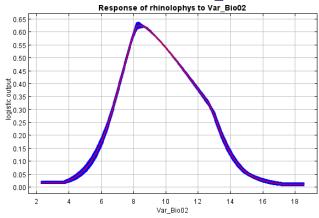
### Model responses

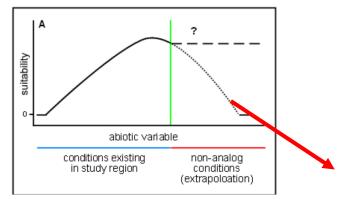
- MAXENT provides a univariate probability response plot
- These show howprobability varies according to each environmental factor
- You can explore these outputs to know if you're model was trained close to the limits of the species range

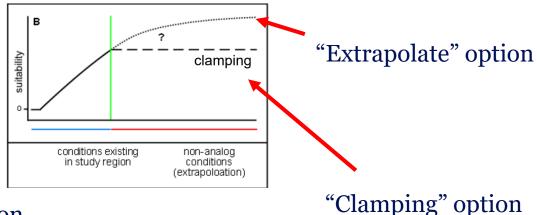
### Clamping:

• Tells MAXENT what to do when the variable is outside the training range

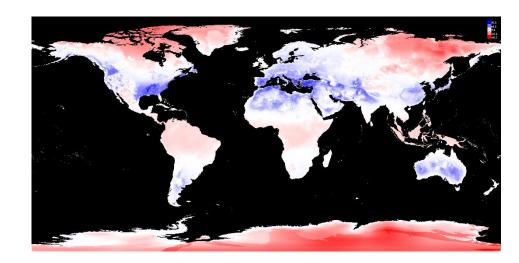
### Good example!

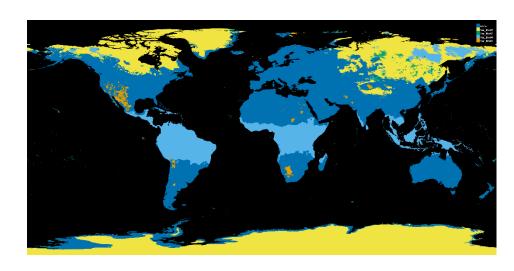






- Algorithms described in: (<u>Elith,2010</u>; <u>Supporting information</u>)
- Multivariate Environmental Similarity Surfaces (MESS)
  - Produces a map estimating the similarity [-100, 100];
  - With o being "equal" and -100 or 100 being totally (negatively or positively) dissimilar
- Most Dissimilar Variables (MoD)
  - Maps which of the various environmental had the most dissimilar MESS for that particular location
- These models should be used to identify regions where we should be suspicious of our model performance
  - Notice: Clamping might (will) affect these surfaces!





#### • Variable importance:

- These provide an estimate of how significant X variable was for the MAXENT model
- Critical for ecologists: These are the variables "driving" the function that defines the distribution of the species.

#### Percent contribution:

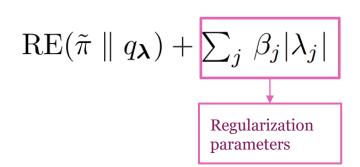
- Δ changes in AUC gain based on Regularization parameters "remember the formula"
- Each scalar is in function of each variable, so this is used to measure is contribution

#### • Permutation importance:

- Changes in training AUC by excluding/including the given variable
- And then normalizes, to provide a % of contribution

#### Take note:

- % contribution ≈ Permutation importance is a Good sign
- These estimates are highly affected by autocorrelation between environmental variables

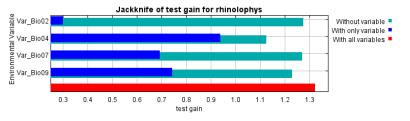


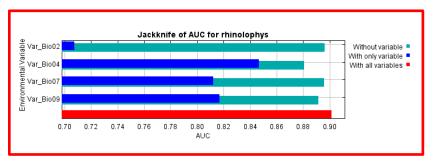
Variable	Percent contribution	Permutation importance
_Bio04	52.9	50.8
_Bio12	36.3	31.9
_Bio01	6.6	12.9
_Bio15	3.2	2.6
_Bio19	1.1	1.9

#### Jacknife testing

- Asses the variation in accuraccy (aka, gain or AUC) if a model is ran using only variable X or excluding variable X "jacknife"
- The "non-used" variables are set to the mean value of the distribution
- Mostly the same information as variable importance
  - Remember: Ecologists should care for what drives the distribution
- MAXENT provides 3 versions:
  - Based on the training acuraccy gain
  - Based on the test accuraccy gain (data that was left out!)
  - Based on the AUC <- This is the most helpful as it relates directly with the AUC-ROC report







### • In summary:

- Non-analogous conditions how to deal with them?
- Species with unstable niche (e.g. exotic species) often break the assumptions of Hutchinson niche theory

### MAXENT diagnostic's:

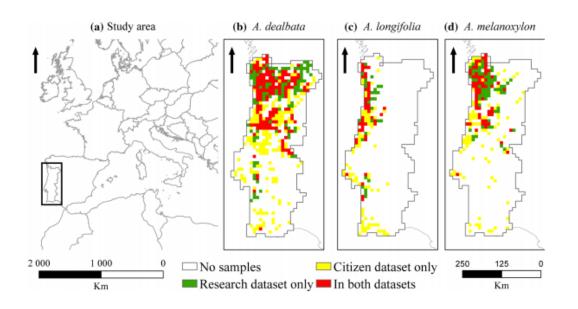
- Response curves -> Indication of how your model responds to the environmental variable
- MESS & MoD -> Indication of where and why is your mode extrapolating
- Variable importance -> indication of which variables are more important for the species distributions
- Jacknife testing -> Same as above
- Your model performance should be interpreted using all the diagonostics offered:
  - Otherwise.. You might find yourself predicting giraffes in the artic

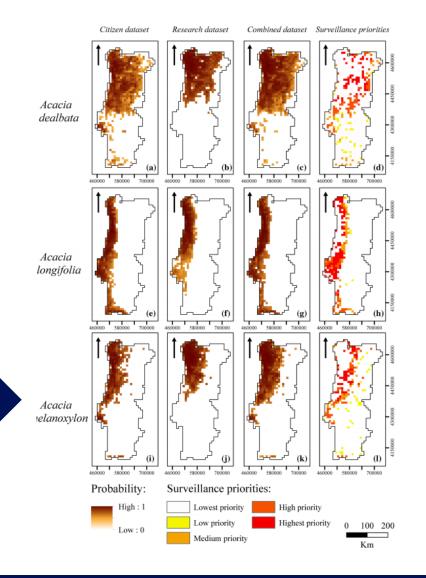
# Two case studies:

**Shameless self promotion!** 

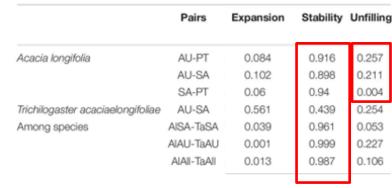


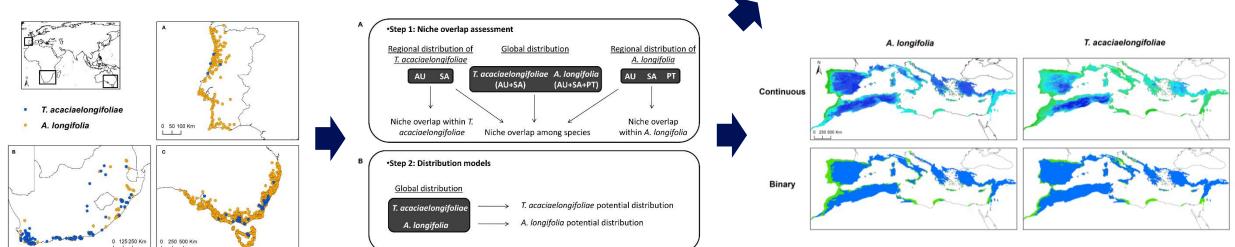
- Using Citizen science to improve SDM (<u>César de Sá</u>, 2019)
  - Compared how data from citizens coupled with scientific surveys improves SDM coverage for invasive alien species
  - Identified areas of highest surveillance priority (aka likelihood of invasion but no data is available:





- Predicting the distribution of a biocontrol agent introduced in Portugal (<u>Dinis</u>, <u>2020</u>)
  - The first biocontrol introduction in continental europe!
  - Measured niche overlap to assess if there is significant change & predicted its distribution





# Thank you!

# Q&A time



In the afteroon, you get to try this on your SPECIES!

# Setting up MAXENT & JAVA

And starting by Downloading the climate data during lunch



### Setting up Java

#### 1. For Java:

- 1. Go to <a href="https://www.java.com/en/download/help/download\_options.xml">https://www.java.com/en/download/help/download\_options.xml</a>
- 2. Follow the steps to download and install the software for your operating system
- 3. Unsure about your OS? In windows, go to your system properties:

#### 2. Check Java installation:

- 1. Go to the search box and write "Command line" (or in your own OS language)
- 2. On the DOS box that opens, type: java version

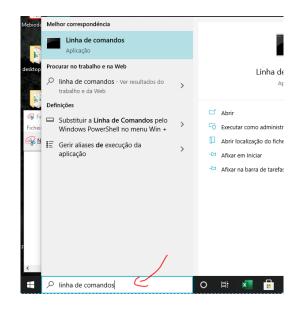
```
Microsoft Windows [Version 10.0.19041.630]
(c) 2020 Microsoft Corporation. Todos os direitos reservados.

C:\Users\Nuno>java -version
    java version "1.8.0_271"
    Java(TM) SE Runtime Environment (build 1.8.0_271-b09)
    Java HotSpot(TM) 64-Bit Server VM (build 25.271-b09, mixed mode)

C:\Users\Nuno>
```

3. If all is well, you will have a similar output

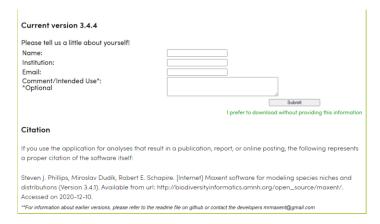


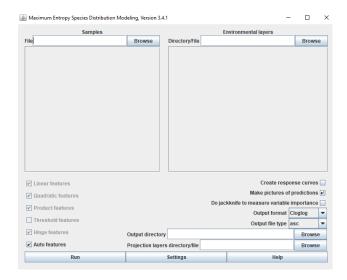


### **Setting up MAXENT:**

- 1. Go to <a href="https://biodiversityinformatics.amnh.org/open\_source/maxent/">https://biodiversityinformatics.amnh.org/open\_source/maxent/</a>
- 2. Tell them a bit about yourself
  - You can lie, but remember it is a sin
- 3. Download the software and unzip it to a folder
- 4. Click on the .Jar file to activate
- 5. If you see the screen, should be fine

PS: Would be nice to cite them on your report





# Downloading the climate data

- 1. Go to the manual
  - It's already in brightspace!
- Follow the steps to download the climate data detailed there

### In summary:

- 1. Go to <a href="https://www.worldclim.org/">https://www.worldclim.org/</a>
- 2. Download:
  - Historical bioclimatic data (bio 5m) at 5 minutes resolution
  - Future scenario bioclimatic data (bc) data: IPSL-CM6A-LR / SSP370