WORKSHOP: theory-driven computational modeling in computational psychiatry with cpm

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EBERHARD KARLS UNIVERSITÄT TÜBINGEN

Developmental Computational Psychiatry lab

Computational Psychiatry Modeling

House Keeping

9:00 – 10:30

Model building, fitting, and model recovery

BREAK

10:30 – 11:00

11:30 – 13:00

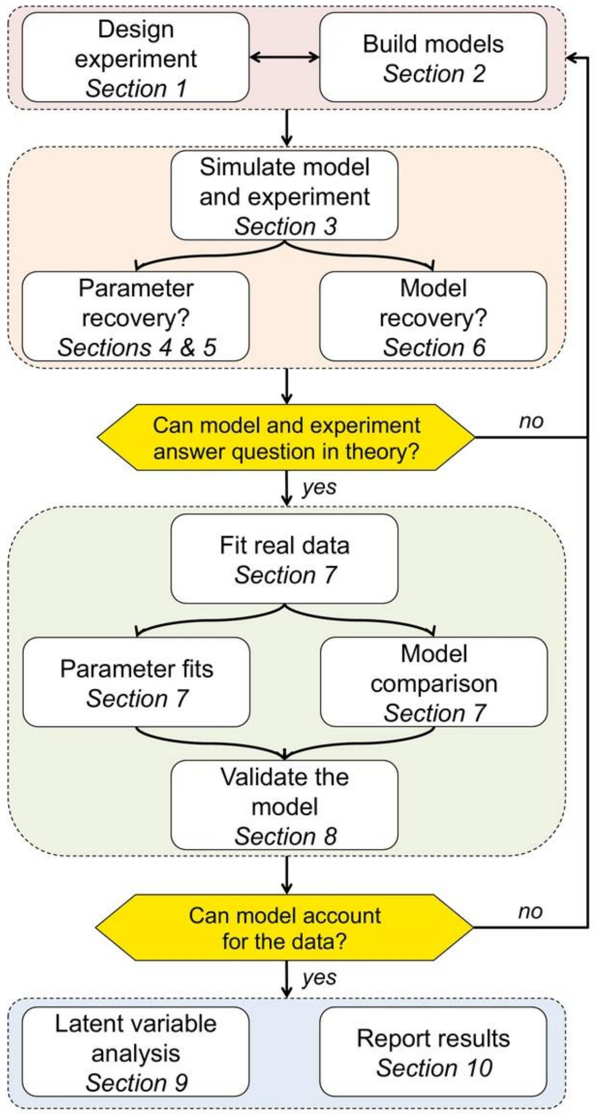
Model comparison, overfitting, model recovery, hierarchical fitting, wrap up!

Workshop outcomes

- Build models
- Evaluate your models prior to data
- Being able to fit the model to data
- Understand the principles of hierarchical modeling
- Evaluate parameter identifiability
- Understand how to evaluate model distinguishability
- Draw inferences on the group level through estimation of hyperparameters

What do the exercises cover?

1. Build models
2. Simulate with models
3. Recover parameters
4. Recover models (optional homework)
5. Fit real data
6. Parameter fits (+ hierarchical parameter estimation)
7. Exploring parameter estimates



Wilson, R. C., & Collins, A. G. (2019). Ten simple rules for the computational modeling of behavioral data. *eLife*, *8*, e49547. https://doi.org/10.7554/eLife.49547

Activity Format

- Complete worksheets
  - read through the Jupyter Notebooks
  - complete each task in chronological order (they tend to build on each other)
- Self-directed activity
- Help each other when you can!

If you need help or have questions, we are here to assist you!

Introduction

A crash-course on the basic concepts…

Which pizza has more pizza?

- 18 inch?
- 2 x 12 inch?

Pizza problem (Guest & Martin, 2021)

Amount of food per order:

$$\phi_i = N_i \, \pi \, r_i^2,$$

where i is the pizza-order option, N is the number of pizzas. Here is our pairwise decision rule:

$$\omega(\phi_i, \phi_j) = \begin{cases} i, & if\ \phi_i > \phi_j \\ j, & otherwise \end{cases}$$


Fermat's Library
@fermatslibrary

Here's a useful counterintuitive fact: one 18 inch pizza has more 'pizza' than two 12 inch pizzas

Pizza problem (Guest & Martin, 2021)

Amount of food per order:

$$\phi_i = N_i \, \pi \, r_i^2,$$

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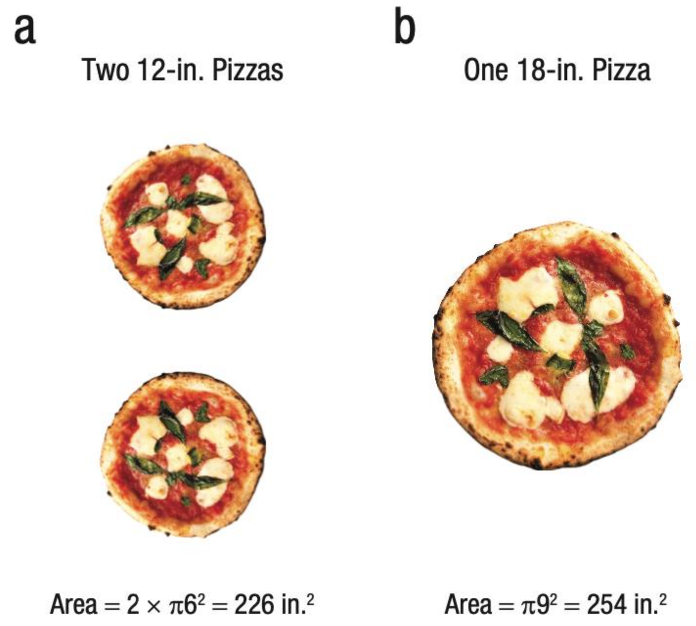
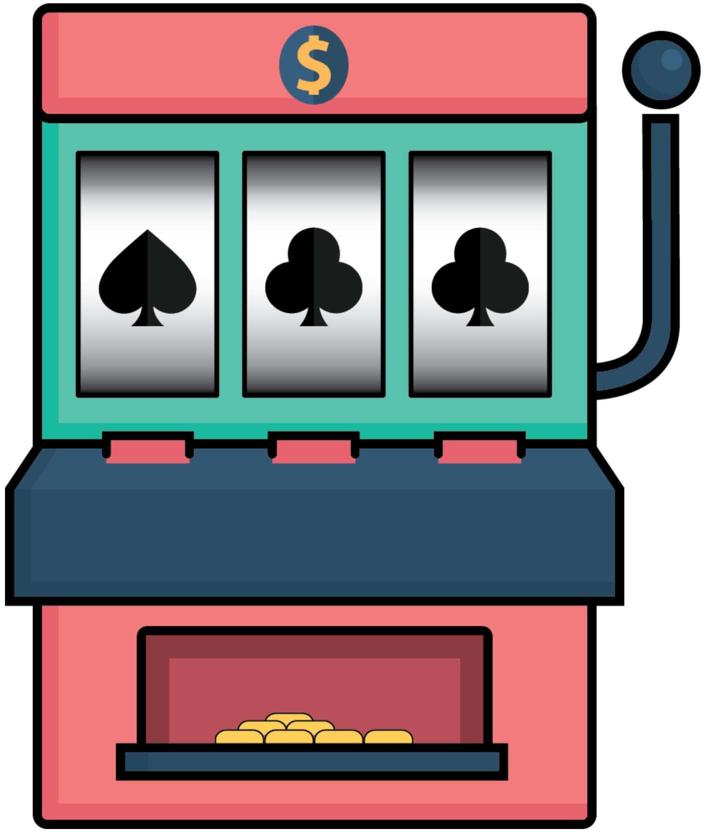
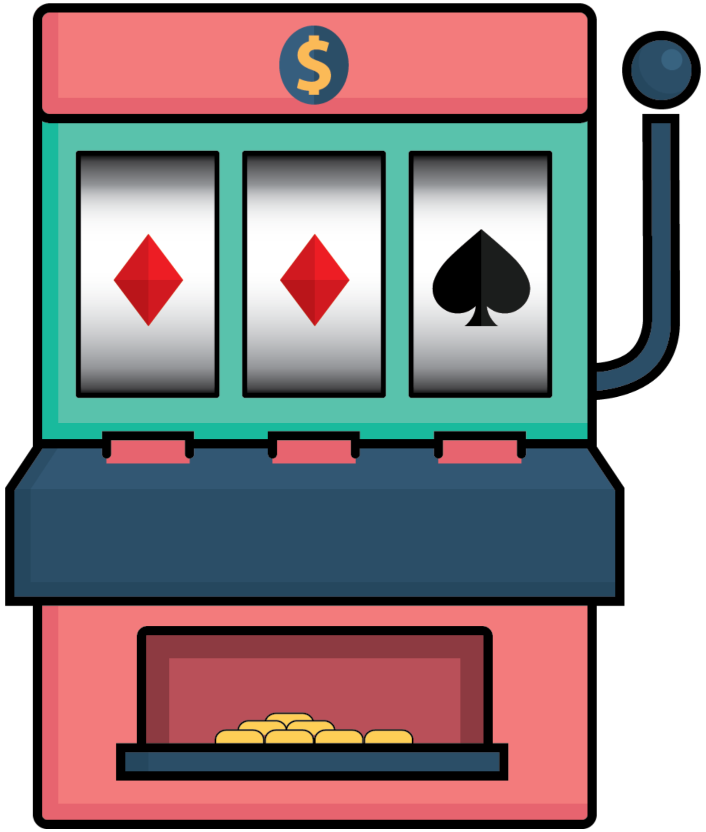


Fig. 1. The pizza problem. Something like comparing the two options presented here can appear counterintuitive, although we all learn the formula for the area of a circle in primary school. Compare (a) two 12-in. pizzas and (b) one 18-in. pizza (all three pizzas are to scale). Which order would you prefer?

Bandit Tasks





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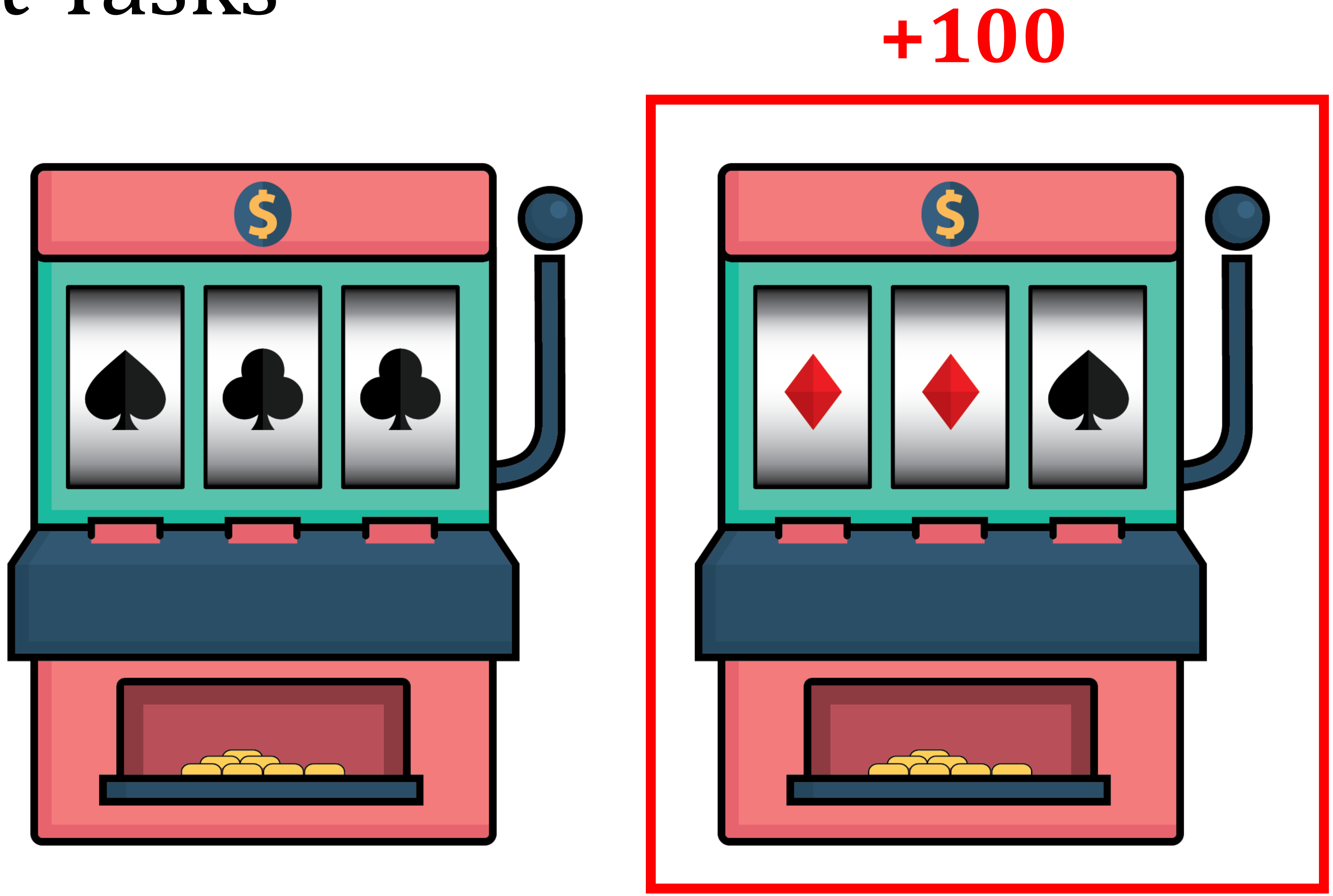

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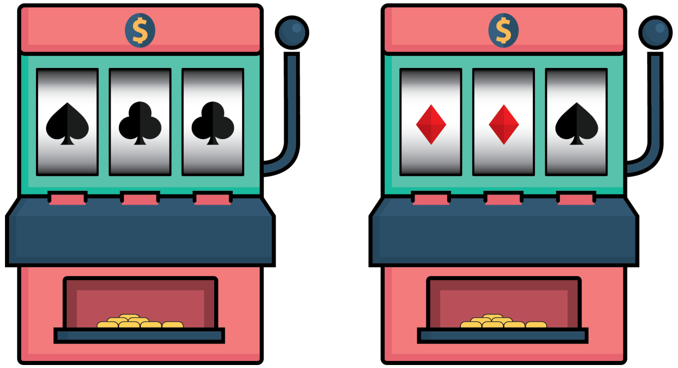
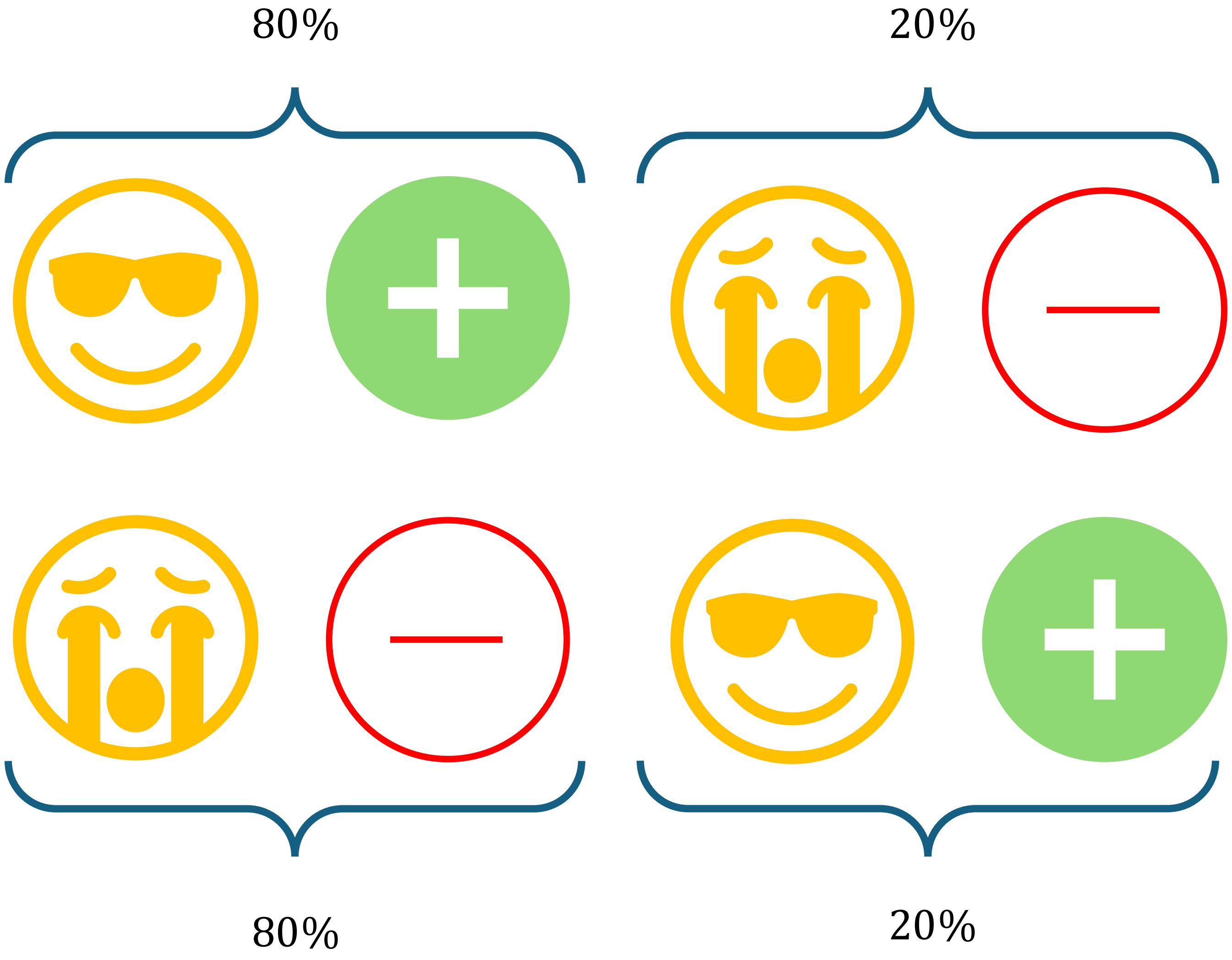




LIVE CODING!

What does the data look like?

Modeling learning in probabilistic environments

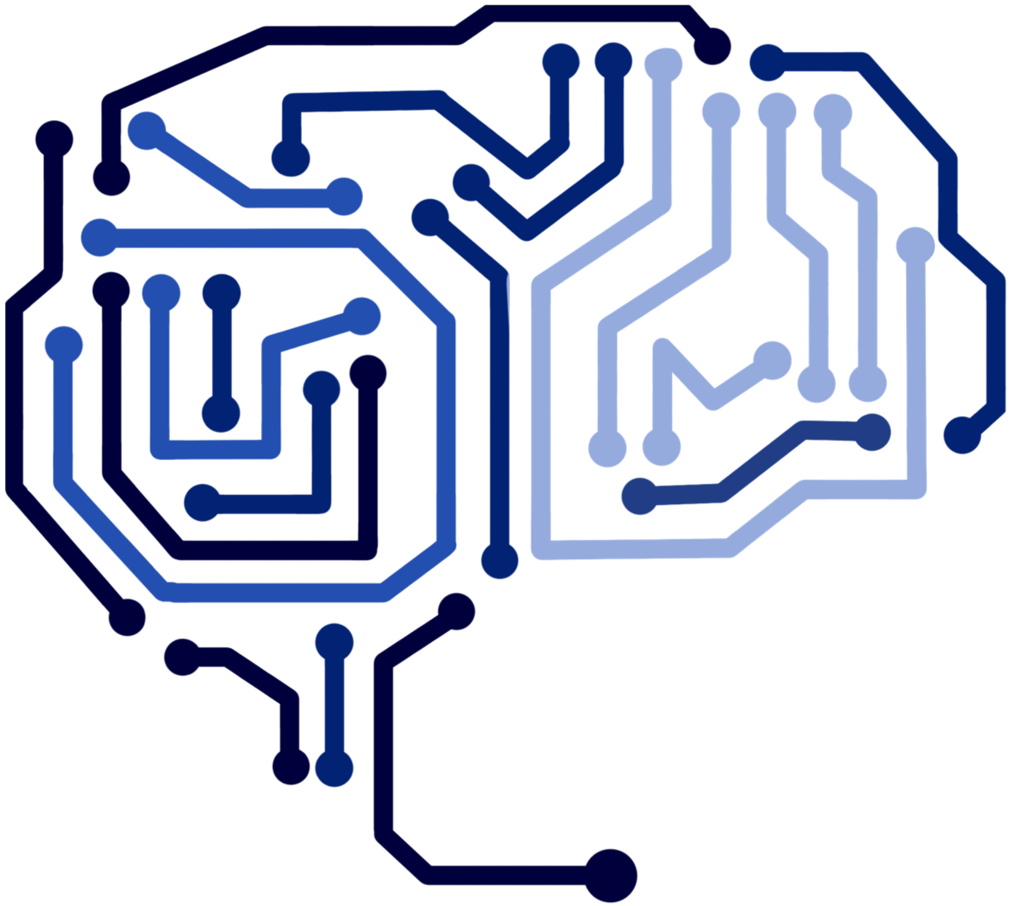
What are the processes we are interested in?

- Learning:
  - **Theoretical Assumption: learning is error-driven**
  - Formula: prediction error (Bush & Mosteller, 1951; Rescorla & Wagner, 1972; McClelland & Rumelhart, 1985; Sutton and Barto, 1981)
  - $\boldsymbol{\alpha}$**: for a learning parameter**
- Decision processes
  - **Theoretical Assumption: idependence from alternatives; simple scalability**
  - Formula: exponential ratio scaling - SoftMax (Bridle, 1990)
  - $\boldsymbol{\beta}$**: inverse temperature**

The *cpm* toolbox

Getting you the tools to get going

Computational Psychiatry Modeling Library in Python 🐍



It is interoperable with widely-used libraries

pandas - a fast, powerful, flexible and easy to use open-source data analysis and manipulation tool

numpy - a fundamental package for scientific computing with Python

The **cpm** modules

cpm.generators

cpm.applications

cpm.optimisation

cpm.hierarchical

cpm.datasets

cpm.models

Where to get the goods

- https://github.com/DevComPsy/cpm
- https://cpm-toolbox.net

pip install cpm-toolbox (stable version)

pip install git+https://github.com/DevComPsy/cpm.git (nightly version)

Model Construction: parameters

cpm.generators.Value

`cpm.generators.Value(value=None, lower=0, upper=1, prior=None, args=None, **kwargs)`

The `Value` class is a wrapper around a float value, with additional details such as the prior distribution, lower and upper bounds. It supports all basic mathematical operations and can be used as a regular float with the parameter value as operand.

Parameters:

- `value` (`float` , default: `None`) – The value of the parameter.
- `lower` (`float` , default: `0`) – The lower bound of the parameter.
- `upper` (`float` , default: `1`) – The upper bound of the parameter.
- `prior` (`string or object` , default: `None`) – If a string, it should be one of continuous distributions from `scipy.stats` . See the scipy documentation for more details. The default is None. If an object, it should be or contain a callable function representing the prior distribution of the parameter with methods similar to `scipy.stats` distributions. See Notes for more details.
- `args` (`dict` , default: `None`) – A dictionary of arguments for the prior distribution function.

Notes

We currently implement the following continuous distributions from `scipy.stats` corresponding to the `prior` argument:

- 'uniform'
- 'truncated_normal'
- 'beta'
- 'gamma'
- 'truncated_exponential'
- 'norm'

Because these distributions are inherited from `scipy.stats` , see the scipy documentation for more details on how to update variables of the distribution.

Returns:

- `Value` – A Value object, where each attribute is one of the arguments provided for the function. It support all basic mathematical operations and can be used as a regular float with the parameter value as operand.

cpm.generators.Parameters

`cpm.generators.Parameters(**kwargs)`

A class representing a set of parameters. It takes keyword arguments representing the parameters with their values and wraps them into a python object.

Parameters:

- `**kwargs` (`dict` , default: `{}`) – Keyword arguments representing the parameters.

Returns:

- `Parameters` – A Parameters object, where each attributes is one of the keyword arguments provided for the function wrapped by the Value class.

Examples:

```
>>> from cpm.generators import Parameters
>>> parameters = Parameters(a=0.5, b=0.5, c=0.5)
>>> parameters['a']
0.1
>>> parameters.a
0.1
>>> parameters()
{'a': 0.1, 'b': 0.2, 'c': 0.5}
```

The Parameters class can also provide a prior.

```
>>> x = Parameters(
>>>     a=Value(value=0.1, lower=0, upper=1, prior="normal", args={"mean": 0.5, "sd": 0.1}),
>>>     b=0.5,
>>>     weights=Value(value=[0.1, 0.2, 0.3], lower=0, upper=1, prior=None),
>>> )
```

```
>>> x.prior(log=True)
-6.5854290732499186
```

We can also sample new parameter values from the prior distributions.

Model Construction: parameters

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complete parameterization

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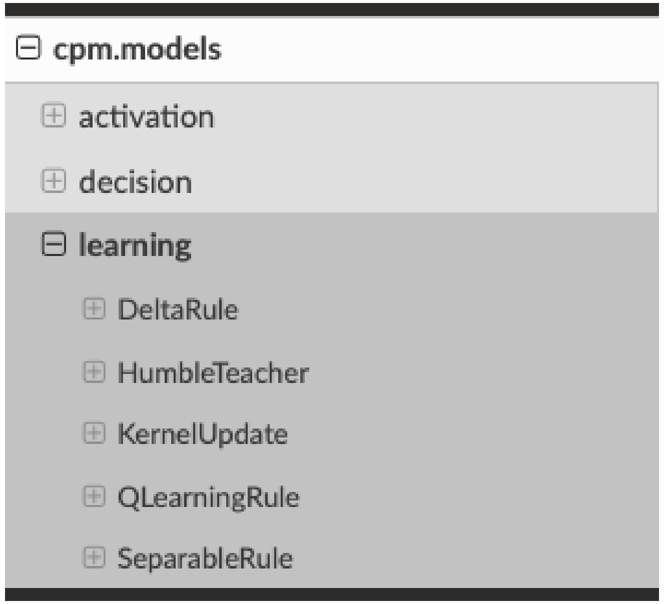
LIVE CODING!

How to specify your parameters?

Model Construction: building your model

- **cpm.models** contain a library of algorithmic components.



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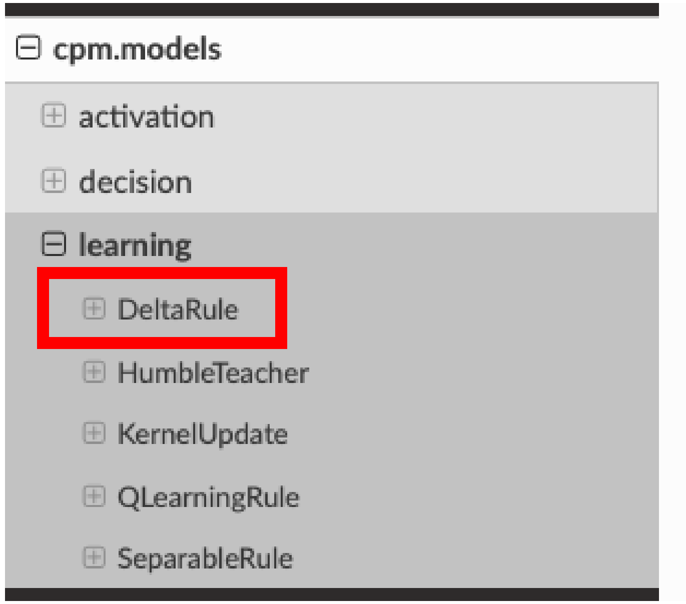

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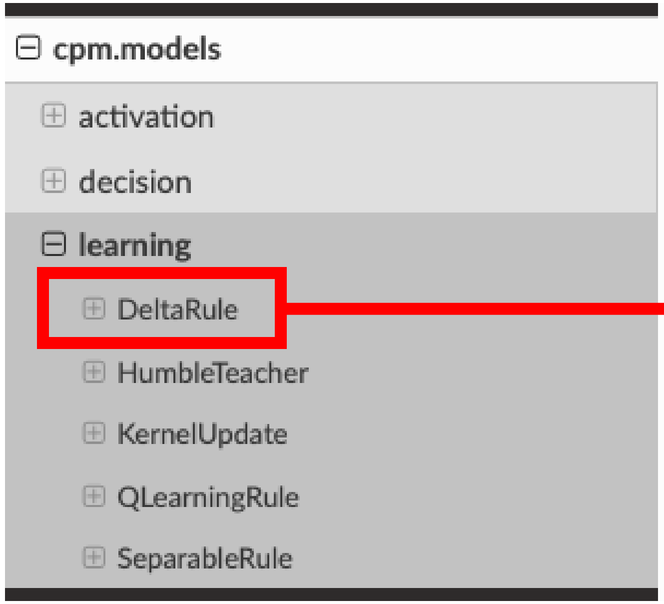

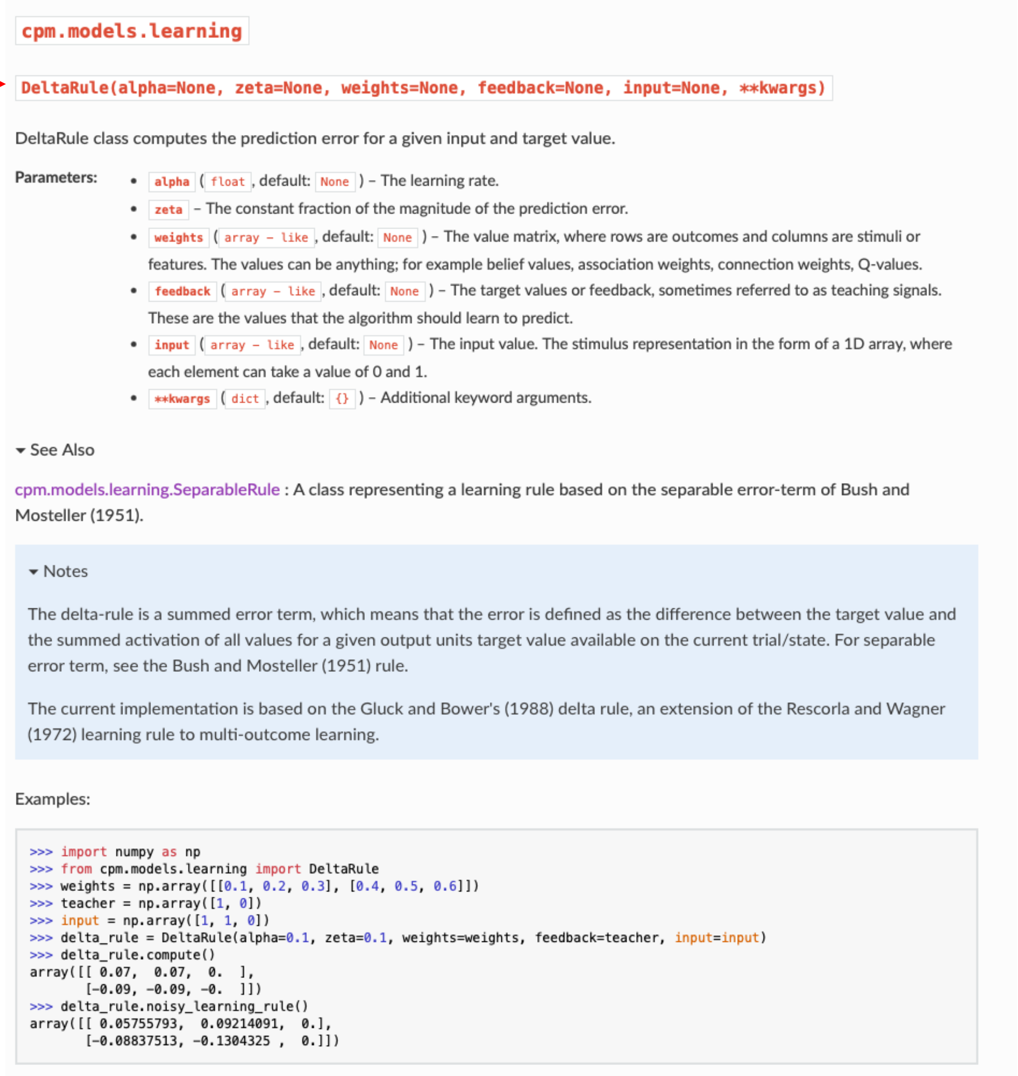

`cpm.models.learning`

`DeltaRule(alpha=None, zeta=None, weights=None, feedback=None, input=None, **kwargs)`

DeltaRule class computes the prediction error for a given input and target value.

Parameters:

- `alpha` (`float` , default: `None`) – The learning rate.
- `zeta` – The constant fraction of the magnitude of the prediction error.
- `weights` (`array - like` , default: `None`) – The value matrix, where rows are outcomes and columns are stimuli or features. The values can be anything; for example belief values, association weights, connection weights, Q-values.
- `feedback` (`array - like` , default: `None`) – The target values or feedback, sometimes referred to as teaching signals. These are the values that the algorithm should learn to predict.
- `input` (`array - like` , default: `None`) – The input value. The stimulus representation in the form of a 1D array, where each element can take a value of 0 and 1.
- `**kwargs` (`dict` , default: `{}`) – Additional keyword arguments.

See Also

cpm.models.learning.SeparableRule : A class representing a learning rule based on the separable error-term of Bush and Mosteller (1951).

Notes

The delta-rule is a summed error term, which means that the error is defined as the difference between the target value and the summed activation of all values for a given output units target value available on the current trial/state. For separable error term, see the Bush and Mosteller (1951) rule.

The current implementation is based on the Gluck and Bower's (1988) delta rule, an extension of the Rescorla and Wagner (1972) learning rule to multi-outcome learning.

Examples:

```
>>> import numpy as np
>>> from cpm.models.learning import DeltaRule
>>> weights = np.array([[0.1, 0.2, 0.3], [0.4, 0.5, 0.6]])
>>> teacher = np.array([1, 0])
>>> input = np.array([1, 1, 0])
>>> delta_rule = DeltaRule(alpha=0.1, zeta=0.1, weights=weights, feedback=teacher, input=input)
>>> delta_rule.compute()
array([[ 0.07,  0.07,  0.  ],
       [-0.09, -0.09, -0.  ]])
>>> delta_rule.noisy_learning_rule()
array([[ 0.05755793,  0.09214091,  0.],
       [-0.08837513, -0.1304325 ,  0.]])
```

LIVE CODING!

How to specify your model?

EXERCISES

EXERCISE 1.1A and EXERCISE 1.1B

- EXERCISE 1.1A: create model parameters (doing it together)
  - LINKS to docs
- EXERCISE 1.1B: create model implementation
  - Specify the learning process: single linear operator cpm.models.learning.SeperableRule
  - Specify the decision process: exponential ratio scaling cpm.models.decision.Softmax

Model Construction: taking in your specification and applying it to trial-level data

cpm.generators

- **cpm.generators.Parameters, cpm.generators.Value**
- **cpm.generators.Wrapper** (turns model parameterization and model function in a fully-fledged model)
- **cpm.generators.Simulator** (simulates data for multiple participants)

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`cpm.generators.Wrapper(model=None, data=None, parameters=None)`

A `Wrapper` class for a model function in the CPM toolbox. It is designed to run a model for a **single** experiment (participant) and store the output in a format that can be used for further analysis.

Parameters:

- **model** (`function`, default: `None`) – The model function that calculates the output(s) of the model for a single trial. See Notes for more information. See Notes for more information.
- **data** (`DataFrame or dict`, default: `None`) – If a `pandas.DataFrame`, it must contain information about each trial in the experiment that serves as an input to the model. Each trial is a complete row. If a `dictionary`, it must contains information about the each state in the environment or each trial in the experiment - all input to the model that are not parameters.
- **parameters** (`Parameters object`, default: `None`) – The parameters object for the model that contains all parameters (and initial states) for the model. See Notes on how it is updated internally.

Returns:

- **Wrapper** (`object`) – A Wrapper object.

▾ Notes

The model function should take two arguments: `parameters` and `trial`. The `parameters` argument should be a Parameter object specifying the model parameters. The `trial` argument should be a dictionary or `pd.Series` containing all input to the model on a single trial. The model function should return a dictionary containing the model output for the trial. If the model is intended to be fitted to data, its output should contain the following keys:

- 'dependent': Any dependent variables calculated by the model that will be used for the loss function.

If a model output contains any keys that are also present in parameters, it updates those in the parameters based on the model output.

Information on how to compile the model can be found in the [Tutorials - Build your model][/tutorials/defining-model] module.

Model Construction: taking in your specification and applying it to trial-level data

cpm.generators

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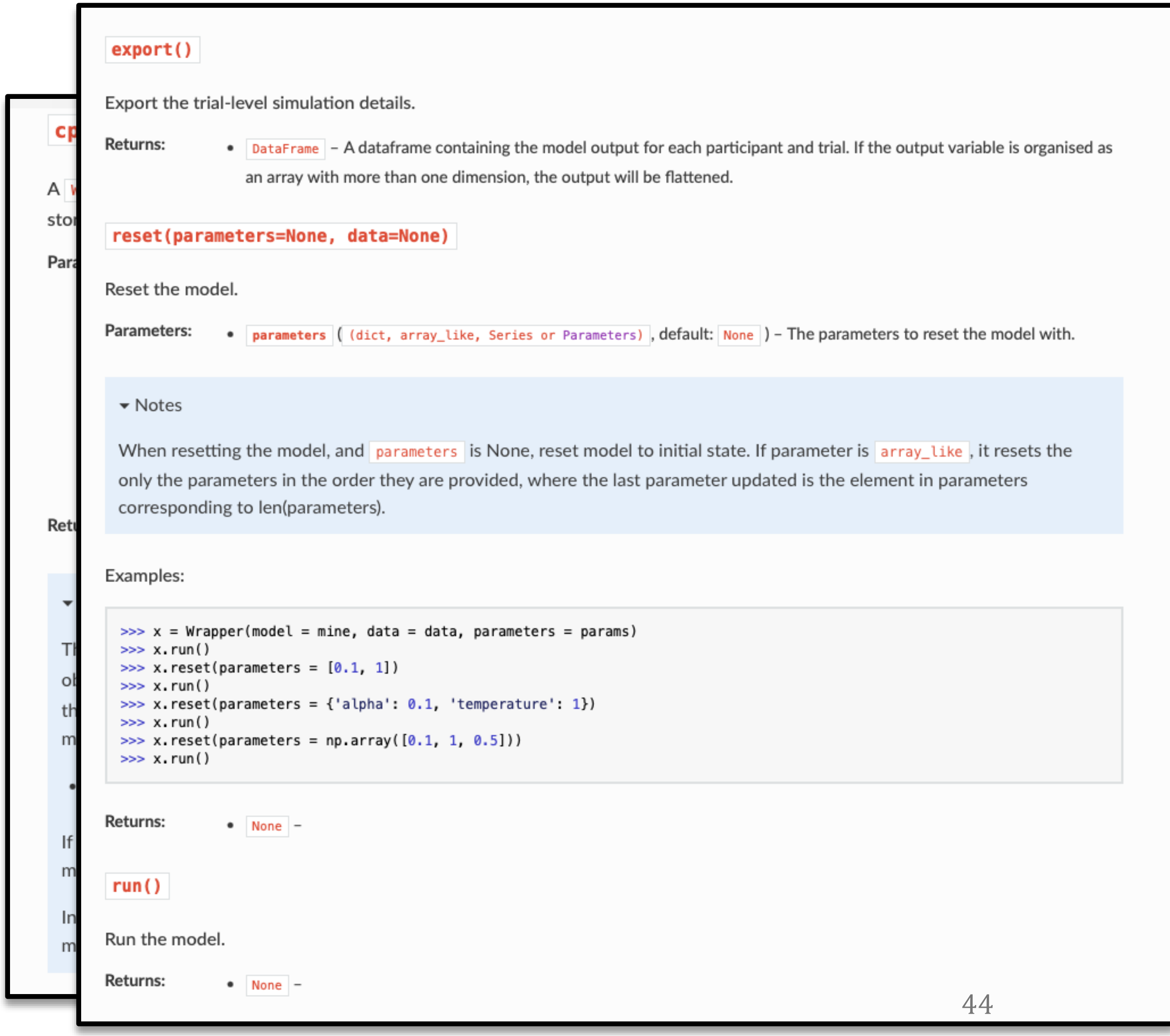


`export()`

Export the trial-level simulation details.

Returns:
- `DataFrame` – A dataframe containing the model output for each participant and trial. If the output variable is organised as an array with more than one dimension, the output will be flattened.

`reset(parameters=None, data=None)`

Reset the model.

Parameters:
- `parameters` (`(dict, array_like, Series or Parameters)`, default: `None`) – The parameters to reset the model with.

▾ Notes

When resetting the model, and `parameters` is None, reset model to initial state. If parameter is `array_like`, it resets the only the parameters in the order they are provided, where the last parameter updated is the element in parameters corresponding to len(parameters).

Examples:

```
>>> x = Wrapper(model = mine, data = data, parameters = params)
>>> x.run()
>>> x.reset(parameters = [0.1, 1])
>>> x.run()
>>> x.reset(parameters = {'alpha': 0.1, 'temperature': 1})
>>> x.run()
>>> x.reset(parameters = np.array([0.1, 1, 0.5]))
>>> x.run()
```

Returns:
- `None` –

`run()`

Run the model.

Returns:
- `None` –

LIVE CODING!

EXERCISE 1.2

- What effect do parameters have on model behaviour?

1. Pick three learning rate parameters.
2. Run the model and look at the plots.
3. Repeat step 1 and 3 until you think the different parameters produce **distinctly different** model behaviour.

EXERCISE 1.2

- What effect do parameters have on model behaviour?

Questions:

What do you notice here? What do you think about the model's behaviour?
How do the parameters affect the model's predictions?
How do the initial Q-values affect the model's predictions?
Anything that surprises you?

Model Construction: simulating data

cpm.generators

- **cpm.generators.Parameters, cpm.generators.Value**
- **cpm.generators.Wrapper** (turns model parameterization and model function in a fully-fledged model)
- **cpm.generators.Simulator** (simulates data for multiple participants)

`cpm.generators.Simulator(wrapper=None, data=None, parameters=None)`

A `Simulator` class for a model in the CPM toolbox. It is designed to run a model for **multiple** participants and store the output in a format that can be used for further analysis.

Parameters:

- `wrapper` (`Wrapper` , default: `None`) – An initialised Wrapper object for the model.
- `data` (`pandas.core.groupby.generic.DataFrameGroupBy or list of dictionaries` , default: `None`) – The data required for the simulation. If it is a pandas.core.groupby.generic.DataFrameGroupBy, as returned by `pandas.DataFrame.groupby()` , each group must contain the data (or environment) for a single participant. If it is a list of dictionaries, each dictionary must contain the data (or environment) for a single participant.
- `parameters` (`(Parameters, DataFrame, Series or list)` , default: `None`) – The parameters required for the simulation. It can be a Parameters object or a list of dictionaries whose length is equal to data. If it is a Parameters object, Simulator will use the same parameters for all simulations. It is a list of dictionaries, it will use match the parameters with data, so that for example parameters[6] will be used for the simulation of data[6].

Returns:

- `simulator` (`Simulator`) – A Simulator object.

`export(save=False, path=None)`

Return the trial- and participant-level information about the simulation.

Parameters:

- `save` (`bool` , default: `False`) – If True, the output will be saved to a file.
- `path` (`str` , default: `None`) – The path to save the output to.

Returns:

- `DataFrame` – A dataframe containing the the model output for each participant and trial. If the output variable is organised as an array with more than one dimension, the output will be flattened.

`generate(variable='dependent')`

Generate data for parameter recovery, etc.

Parameters:

- `variable` – Name of the variable to pull out from model output.

LIVE CODING!

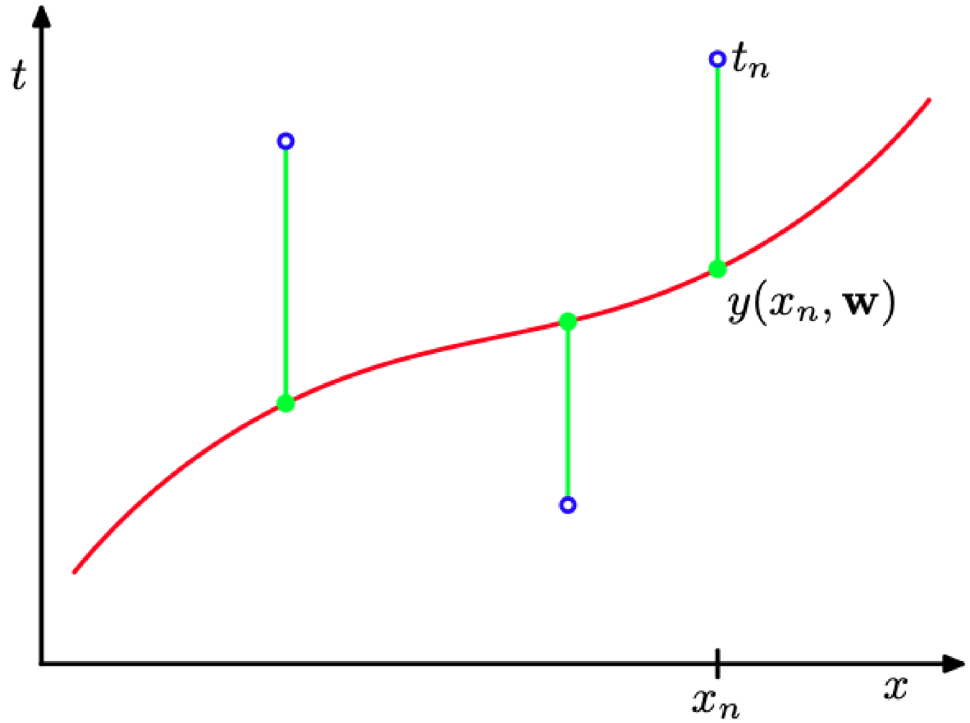
Discrepancy (error) functions: *comparing model output to experimental observations*

- What is the problem here?
- We have a set of values recorded in the experiment, the data: Y
- We have a set of values produced by the model, the predictions: M

So the question is… how close is M to Y?

Discrepancy (error) functions: *comparing model output to experimental observations*

Figure 1.3 The error function (1.2) corresponds to (one half of) the sum of the squares of the displacements (shown by the vertical green bars) of each data point from the function $y(x, \mathbf{w})$.



Bishop, C. M. (2006). *Pattern recognition and machine learning*. Springer.

Discrepancy (error) functions: non-parametric functions

- Sum of Squared Errors (SSE)
- Root Mean Squared Deviations (RMSD)
- χ^2 (chi-square)
- G^2 (log-likelihood ratio)

- $SSE = \sum_{j=1}^{J}(y_j - m_j)^2$
- $RMSD = \sqrt{\frac{\sum_{j=1}^{J}(y_j - m_j)^2}{J}}$
- $\chi^2 = \sum_{j=1}^{J}\frac{(y_j - Nm_j)^2}{Nm_j}$
- $G^2 = 2\sum_{j=1}^{J} log\left(y_j \log\frac{y_j}{Nm_j}\right)$

Discrepancy functions: likelihoods

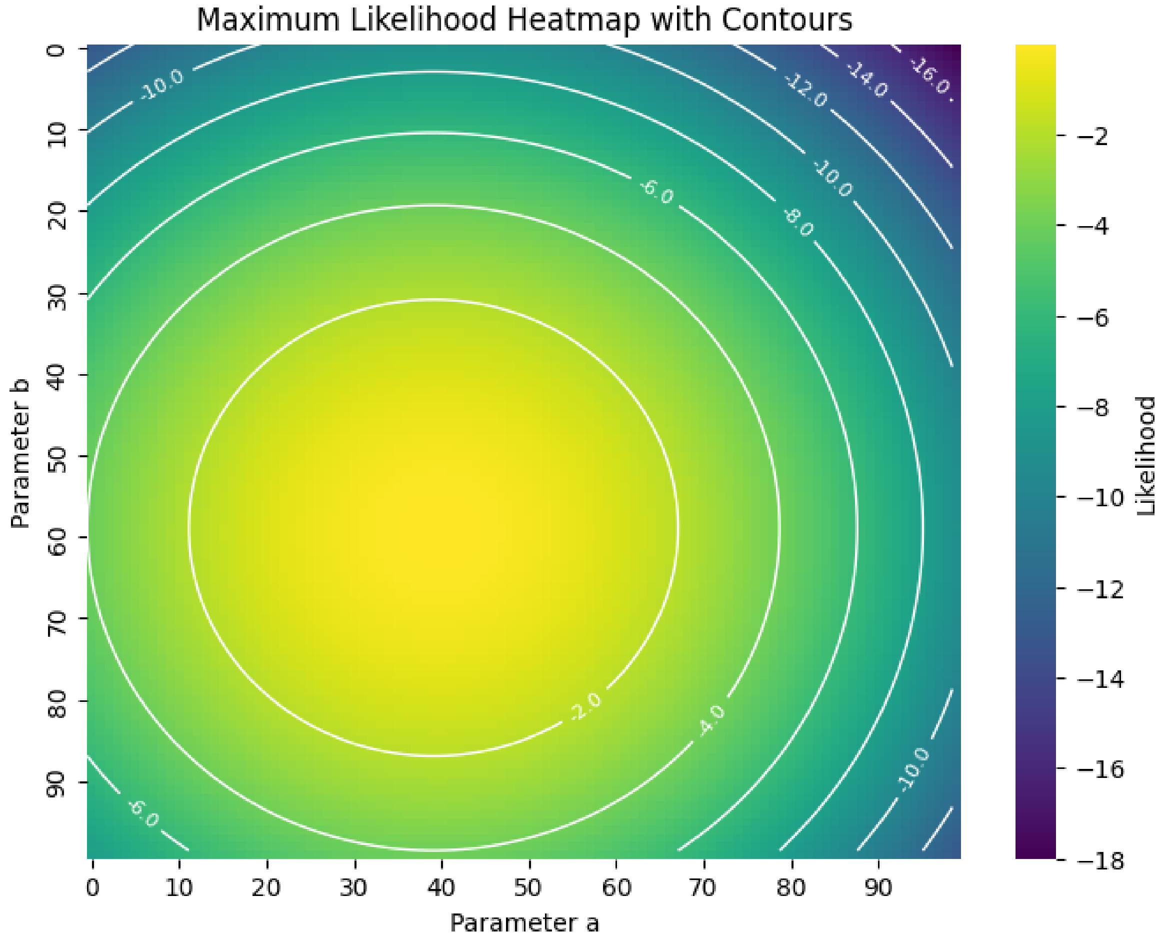
- (most) Models will assign a probability, p_j, for each outcome, y_j
- p_j is the mean of a probability distribution
- p and y can be related through the function, f

These measures are coniditonal on the (M) model and its current (θ) parameter set:

$$f(y \mid \theta, M)$$

Parameter estimation: maximum likelihood estimation

We are often not concerned about all possible parameter values… only about the best-fitting parameters.



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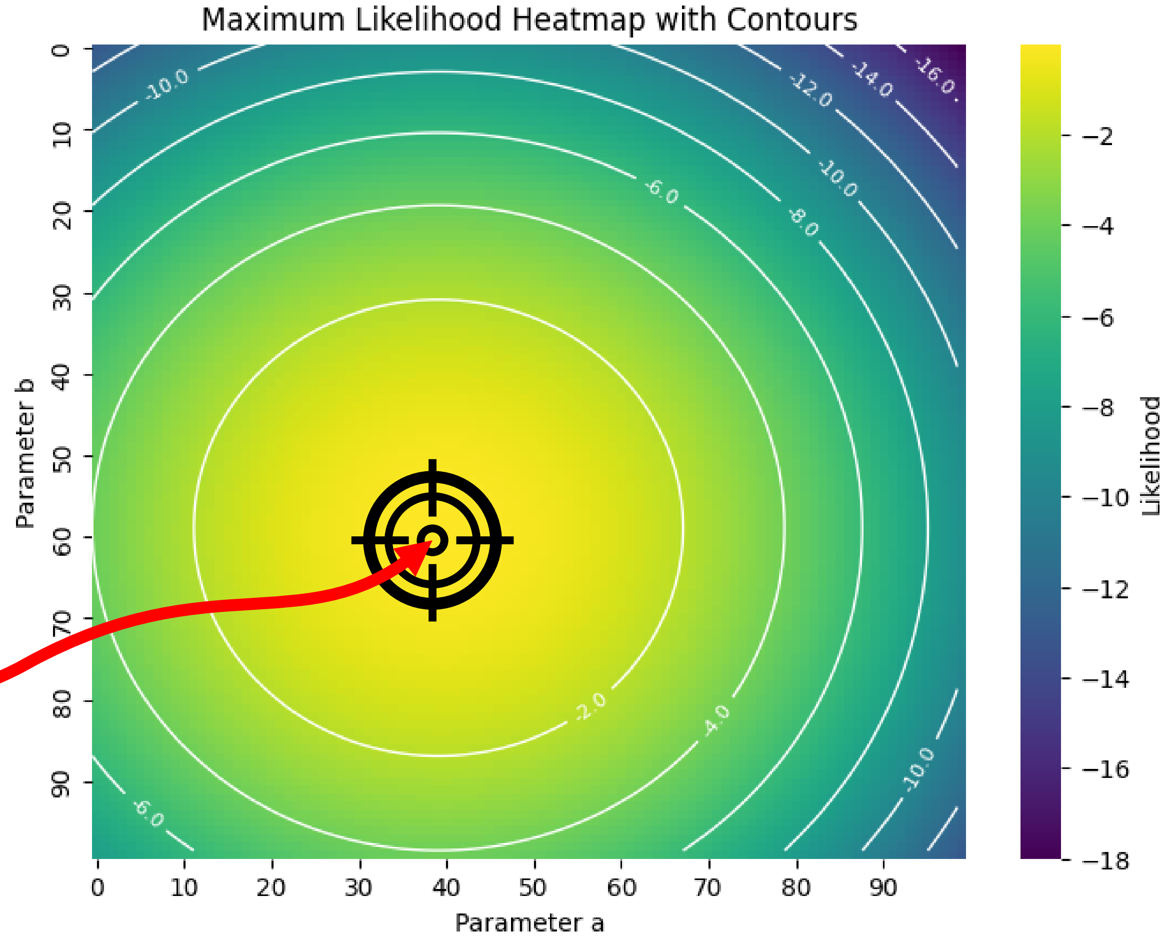


Parameter Estimation

Most parameter estimation techniques requires us to minimize our likelihood (objective) function:

$$\ln L(y_j|\theta) = -\sum_{j=1}^{N} \log\left[P\left(y_j\middle|\theta\right)\right]$$

Parameter Estimation

The goal of parameter estimation is to find the parameters that maximise the agreement between the model and the data.

- Models that approximate the data well can tell you something about the utility of a model.

Parameter Estimation (caveats)

So, what doesn’t it tell you? (Roberts & Pashler, 2000)

- The flexibility (how much data the model cannot fit?)
- The variability of the data (e.g. diagnosticity, how firmly the data rule out what the theory cannot fit)
- The likelihood of other outcomes (perhaps the theory could have fit any possible results)

Our belief in a model should require all of these aspects

Fitting models to data

- cpm.optimisation (interface to parameter estimation techniques from scipy and other libraries)
  - Fmin
  - FminBound
  - BADS (Bayesian Adaptiove Direct Search)
  - DifferentialEvolultion
  - Minimse
- cpm.optimisation.minimise (a battery of discrepency functions)
  - e.g. LogLikelihoods
  - e.g. Non-parametric functions

Fitting models to data

```
cpm.optimisation.FminBound(model=None, data=None, initial_guess=None, number_of_starts=1, minimisation=None, cl=None, parallel=False, libraries=['numpy', 'pandas'], prior=False, ppt_identifier=None, display=False, **kwargs)
```

Class representing the Fmin search (bounded) optimization algorithm using the L-BFGS-B method.

Parameters:

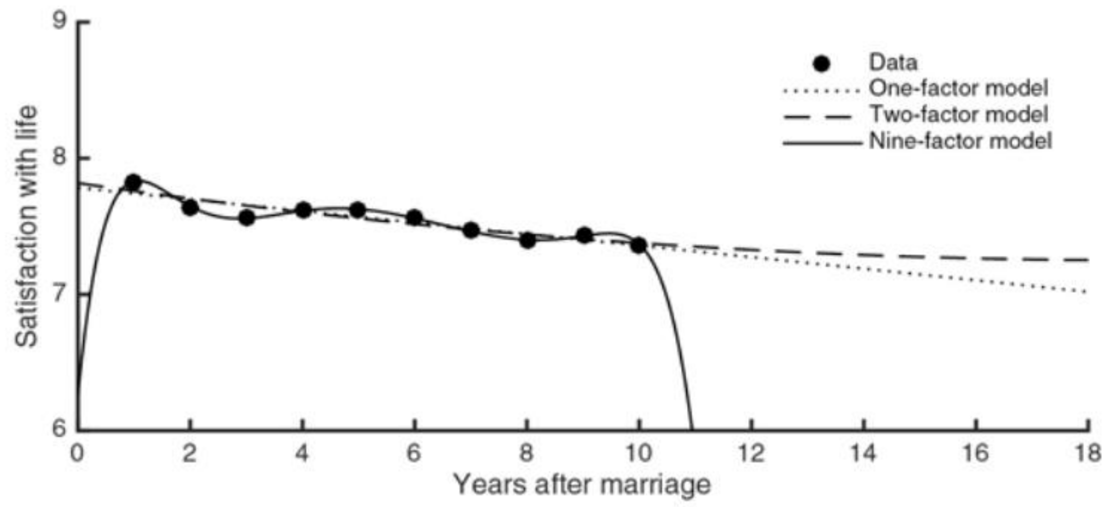
- `model` (`Wrapper`, default: `None`) – The model to be optimized.
- `data` (`(DataFrame, DataFrameGroupBy, list)`, default: `None`) – The data used for optimization. If a pd.Dataframe, it is grouped by the `ppt_identifier`. If it is a pd.DataFrameGroupby, groups are assumed to be participants. An array of dictionaries, where each dictionary contains the data for a single participant, including information about the experiment and the results too. See Notes for more information.
- `minimisation` (`function`, default: `None`) – The loss function for the objective minimization function. See the `minimise` module for more information. User-defined loss functions are also supported.
- `prior` – Whether to include the prior in the optimization. Default is `False`.
- `number_of_starts` (`int`, default: `1`) – The number of random initialisations for the optimization. Default is `1`.
- `initial_guess` (`list or array – like`, default: `None`) – The initial guess for the optimization. Default is `None`. If `number_of_starts` is set, and the `initial_guess` parameter is 'None', the initial guesses are randomly generated from a uniform distribution.
- `parallel` (`bool`, default: `False`) – Whether to use parallel processing. Default is `False`.
- `cl` (`int`, default: `None`) – The number of cores to use for parallel processing. Default is `None`. If `None`, the number of cores is set to 2. If `cl` is set to `None` and `parallel` is set to `True`, the number of cores is set to the number of cores available on the machine.
- `libraries` (`list`, default: `['numpy', 'pandas']`) – The libraries to import for parallel processing for `ipyparallel` with the IPython kernel. Default is `["numpy", "pandas"]`.
- `ppt_identifier` (`str`, default: `None`) – The key in the participant data dictionary that contains the participant identifier. Default is `None`. Returned in the optimization details.
- `**kwargs` (`dict`, default: `{}`) – Additional keyword arguments. See the `scipy.optimize.fmin_l_bfgs_b` documentation for what is supported.

built-in functionalities not available elsewhere

LIVE CODING!

Multi-model comparisons: not all models created equal

The problem of overfitting: *the model fits the training data really well but may perform poorly for independent data (out-of-sample and test dataset)*



Predictions of life satisfaction using models with different numbers of factors.

Christian, B., & Griffiths, T. (2016). *Algorithms to Live By: The Computer Science of Human Decisions*. Henry Holt and Company.

Multi-model comparisons: not all models created equal

This often becomes a problem of complexity

- number of parameters should not approach the number of data points
- results in a push towards parsimony

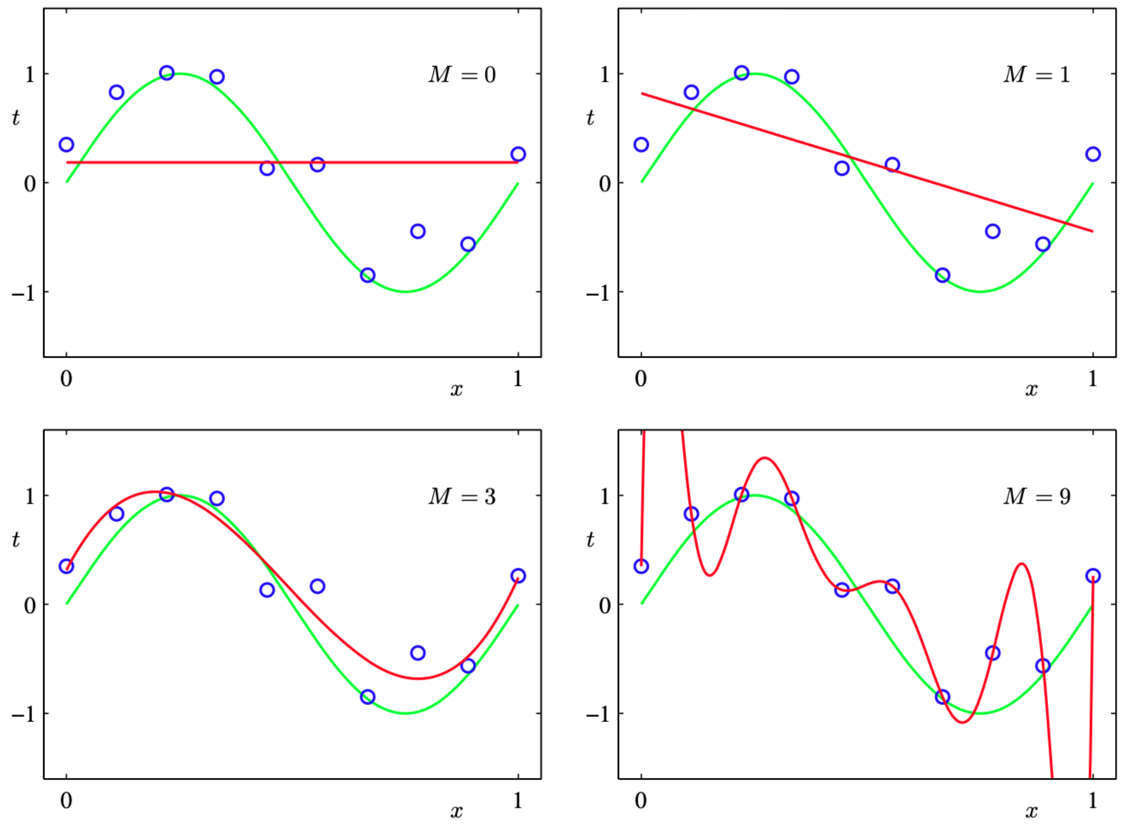


Figure 1.4 Plots of polynomials having various orders M, shown as red curves, fitted to the data set shown in Figure 1.2.

Bishop, C. M. (2006). *Pattern recognition and machine learning*. Springer.

Multi-model comparisons: not all models created equal

Complexity: penalising the number of parameter

- Generalising fit across parameter space (e.g. Bayesian Information or Akaike Information Criterion)
- Incorporating functional form; variance explained by each parameter (e.g. Minimum Description Length, or Bayesian Model Selection)

EXERCISES

EXERCISE 2

- Your job is to estimate model parameters on a small dataset.

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- Your job is to estimate model parameters on a small dataset.

1. What is the difference between the model you fitted first and second?
2. What did you learn about the impact of priors on parameter estimation?
3. What differences you notice between the results of the two parameter estimations? Is it better, worse, or the something else?
4. In what situations would you prefer a hierarchical model over a non-hierarchical one?
5. How confident are you in the parameter estimates, and what could increase your confidence?

Parameter recovery

“Mathematical models often reflect real-world systems and their parameters have biological, chemical, or physical interpretations, and not identifying these parameters can result in ambiguous interpretations.”

Petrica & Popescu (2024)

Parameter recovery

Models often have to satisfy a conditions, called identifiability: *the parameters of a model can be uniquely determined from observed data.*

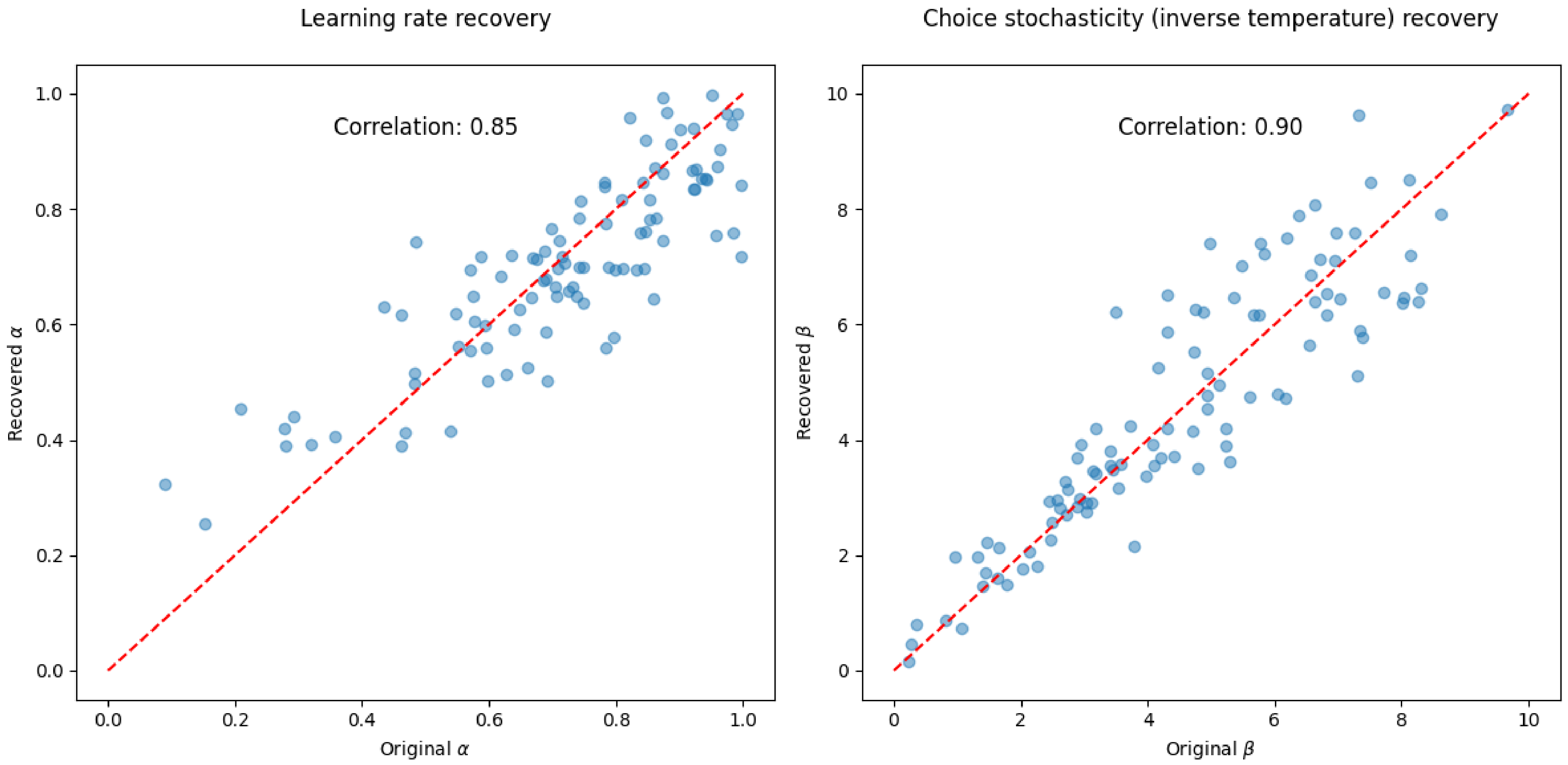
Parameter recovery

Models often have to satisfy a conditions, called identifiability: *the parameters of a model can be uniquely determined from observed data.*

If a parameter **IS IDENTIFIABLE**, given the model and data, there is **only one possible value** for that parameter.

If a parameter **IS NOT IDENTIFIABLE**, given the model and data, there are **multiple possible values** for that parameter.

Parameter recovery



LIVE CODING!

BREAK

11:00 – 11:15

EXERCISE 3

Your job will be to evaluate how identifiable your parameters are with the toolbox.

1. What do you think about the results of the parameter recovery? Are the parameters identifiable?
2. Are there any parameters that are not identifiable? If so, why do you think that is the case?

LIVE CODING!

Model identifiability

Distinguishability: can the experimental design eliminate models?

- Model Recovery (how well models fit each other's genearated data)
- Global model analysis
  - Landscaping
  - Parameter Space Paritioning (also gives information about flexibility/complexity)

Model recovery and confusion matrices

- Determine how identifiable the model is given the experiment (Steyvers et al., 2009)

Predicted Model (model being fitted against the data)

True Model (data generating model)

	Model 1 (M_1)	Model 2 (M_2)	Model 3 (M_2)
Model 1 (M_1)	$P(M_1 \| D_{M_1})$	$P(M_2 \| D_{M_1})$	$P(M_3 \| D_{M_1})$
Model 2 (M_2)	$P(M_1 \| D_{M_2})$	$P(M_2 \| D_{M_2})$	$P(M_3 \| D_{M_2})$
Model 3 (M_3)	$P(M_1 \| D_{M_3})$	$P(M_2 \| D_{M_3})$	$P(M_3 \| D_{M_3})$

Model recovery and confusion matrices

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Model 3 (M_3)	$\mathrm{P}(M_1 \vert D_{M_3})$	$\mathrm{P}(M_2 \vert D_{M_3})$	$\mathrm{P}(M_3 \vert D_{M_3})$

Model recovery and confusion matrices

- Determine how identifiable the model is given the experiment (Steyvers et al., 2009)
- What is it good for?
    - Determine whether you can distinguish between models in your experiment using goodness-of-fit
    - Improve experimental design to distinguish models

Predicted Model (model being fitted against the data)

True Model (data generating model)

	Model 1 (M_1)	Model 2 (M_2)	Model 3 (M_2)
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Model 3 (M_3)	$P(M_1 \| D_{M_3})$	$P(M_2 \| D_{M_3})$	$P(M_3 \| D_{M_3})$

Model recovery and confusion matrices

- Determine how identifiable the model is given the experimen
  2009)
- What is it g
  - Determ
    can dis
    two m
    experi
    goodn
  - Improve experimental design to distinguish models

BEWARE!!!

Confusion matrices (sometimes also called error matrices) mean something slightly different in machine learning. See Opitz, 2024 for a brief review!

Predicted Model (model being fitted against the data)

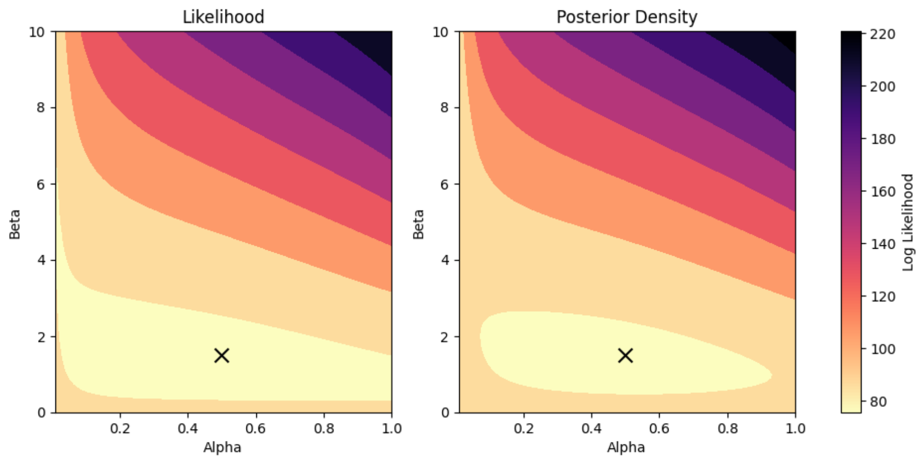
True Model (da
moc

			Model 3 (M_2)
			P(M_3| D_{M_1})
Model 2 (M_2)	P(M_1| D_{M_2})	P(M_2| D_{M_2})	P(M_3| D_{M_2})
Model 3 (M_3)	P(M_1| D_{M_3})	P(M_2| D_{M_3})	P(M_3| D_{M_3})

LIVE CODING!

Hierarchical fitting: model building

- priors are the natural part of **cpm.generators.Parameters**
- priors are defined in the parameterisation of the model
- priors are required



Hierarchical fitting: model building

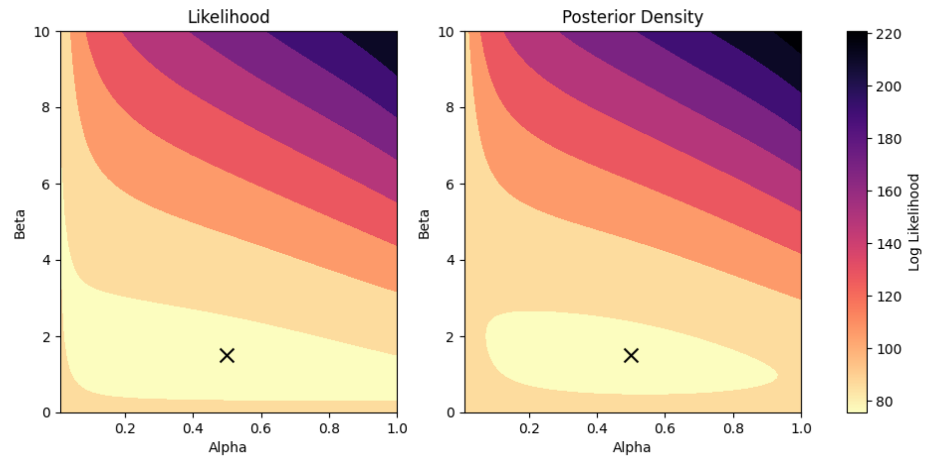
- priors are the natural part of **cpm.generators.Parameters**
- priors are defined in the parameterisation of the model
- priors are required

`cpm.generators.Parameters(**kwargs)`

A class representing a set of parameters. It takes keyword arguments representing the parameters with their values and wraps them into a python object.

Parameters:
- `**kwargs` (`dict`, default: `{}`) – Keyword arguments representing the parameters.

Returns:
- `Parameters` – A Parameters object, where each attributes is one of the keyword arguments provided for the function wrapped by the Value class.



The Parameters class can also provide a prior.

```
>>> x = Parameters(
>>>     a=Value(value=0.1, lower=0, upper=1, prior="normal", args={"mean": 0.5, "sd": 0.1}),
>>>     b=0.5,
>>>     weights=Value(value=[0.1, 0.2, 0.3], lower=0, upper=1, prior=None),
>>> )
```

```
>>> x.prior(log=True)
-6.5854290732499186
```

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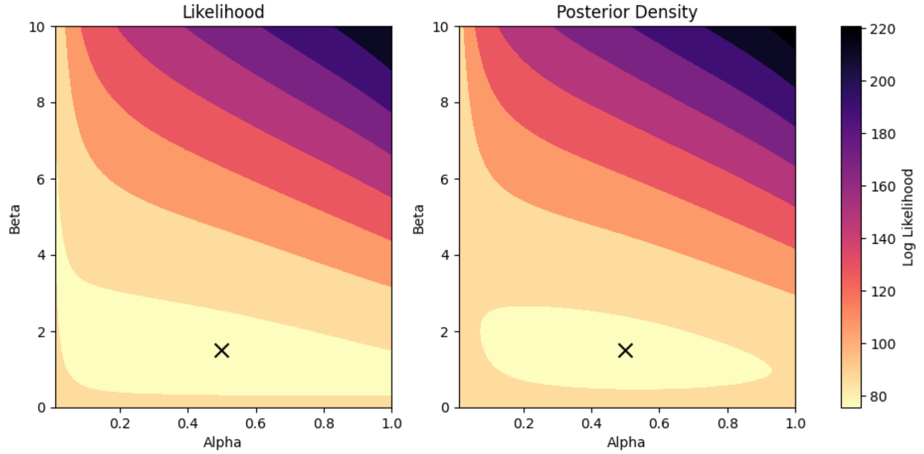

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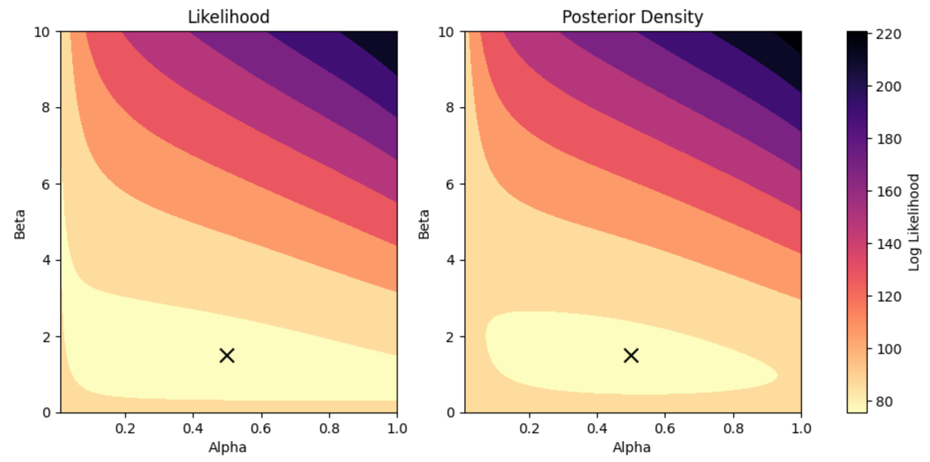

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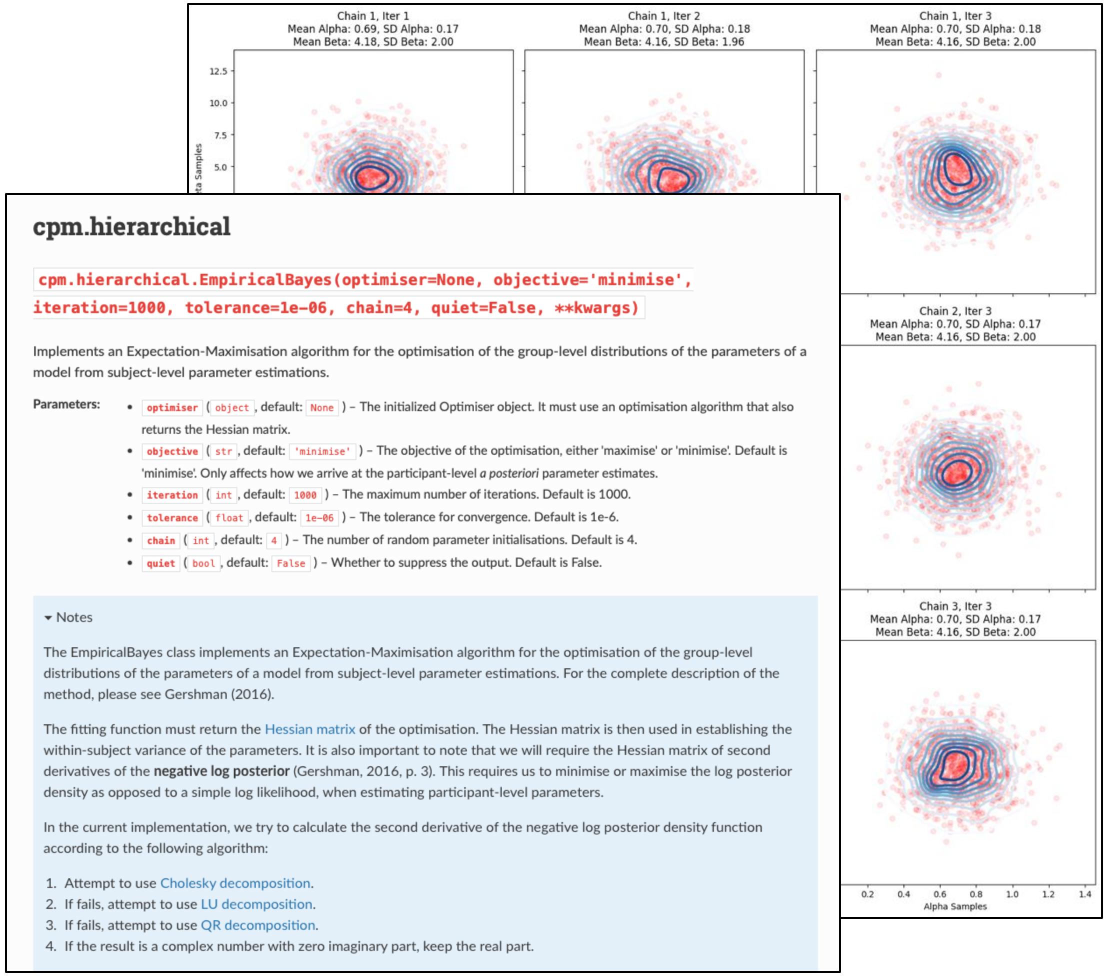
>>> )
```

```
>>> x.prior(log=True)
-6.5854290732499186
```

Hierarchical fitting: hyperparameters



cpm.hierarchical

`cpm.hierarchical.EmpiricalBayes(optimiser=None, objective='minimise', iteration=1000, tolerance=1e-06, chain=4, quiet=False, **kwargs)`

Implements an Expectation-Maximisation algorithm for the optimisation of the group-level distributions of the parameters of a model from subject-level parameter estimations.

Parameters:

- `optimiser` (`object`, default: `None`) – The initialized Optimiser object. It must use an optimisation algorithm that also returns the Hessian matrix.
- `objective` (`str`, default: `'minimise'`) – The objective of the optimisation, either 'maximise' or 'minimise'. Default is 'minimise'. Only affects how we arrive at the participant-level *a posteriori* parameter estimates.
- `iteration` (`int`, default: `1000`) – The maximum number of iterations. Default is 1000.
- `tolerance` (`float`, default: `1e-06`) – The tolerance for convergence. Default is 1e-6.
- `chain` (`int`, default: `4`) – The number of random parameter initialisations. Default is 4.
- `quiet` (`bool`, default: `False`) – Whether to suppress the output. Default is False.

Notes

The EmpiricalBayes class implements an Expectation-Maximisation algorithm for the optimisation of the group-level distributions of the parameters of a model from subject-level parameter estimations. For the complete description of the method, please see Gershman (2016).

The fitting function must return the Hessian matrix of the optimisation. The Hessian matrix is then used in establishing the within-subject variance of the parameters. It is also important to note that we will require the Hessian matrix of second derivatives of the **negative log posterior** (Gershman, 2016, p. 3). This requires us to minimise or maximise the log posterior density as opposed to a simple log likelihood, when estimating participant-level parameters.

In the current implementation, we try to calculate the second derivative of the negative log posterior density function according to the following algorithm:

1. Attempt to use Cholesky decomposition.
2. If fails, attempt to use LU decomposition.
3. If fails, attempt to use QR decomposition.
4. If the result is a complex number with zero imaginary part, keep the real part.

- using priors to constrain parameter estimates
- estimate hyperparameters (means and standard deviations) to draw group-level inferences

cpm.hierarchical

LIVE CODING!

Applications

- the toolbox implements existing models and existing computational methods as a growing number of applications

- cpm.applications.reinforcement_learning.RLRW
- cpm.applications.signal_detection.EstimateMetaD
- (in-development) cpm.applications.reinforcement_learning.MBMF
- (in-development) cpm.applications.decision_making.PTSM
- (in-development) cpm.applications.decision_making.PTSEAM

Other convenient features: modularity

- Functions within their family are interchengeable
- Interaction with third-party libraries

Even more convenience: documentation, examples and troubleshooting!

Wrapping up

Some take-aways and complex topics

What did you do?

✓ 🤖 Build models
(cpm.models, cpm.generators)

✓ 🤔 Evaluate your models prior to data
(cpm.generators, cpm.optimisation)

✓ 😶 🌫️ Evaluate model and parameter identifiability
(cpm.generators, cpm.optimisation)

✓ 📀 Being able to fit the model to data
(cpm.optimisation)

✓ 🧠 Understand the principles of hierarchical modeling
(cpm.generators.Parameters, cpm.hierarchical)

✓ 🎨 Draw inferences on the group level through estimation of hyperparameters
(cpm.hierarchical)

Workshop evaluation form