

Demo: Custom Configurations using ISAconfigurator

Stathis Kanterakis, EBI, 14/03/2013

Motivation

Distributed, data intensive projects often require a precise and consistent collection of metadata from all data sources. Even though ISAcreeator ships with default configurations, data managers may wish to tweak those configurations, add variables they wish to collect or create new configurations from scratch.

This tutorial will guide you through the process of manipulating a simple configuration for a “coin toss” assay. That is, we wish to collect data about how many heads we get tossing coins of different origins, shapes, sizes and materials, in an attempt to see if any of these variables are correlated with whether a coin is fair or not (probability of heads = 0.5).

We will use ISA tools to collect this information.

Requirements

You will need the following:

1. ISAcreeator

- a. Visit <http://isatab.sourceforge.net/tools.html> scroll down and click on your operating system icon under ISAcreeator



- b. Download and unzip the application

2. Our example Coin-toss configuration

- a. Available at <https://bitbucket.org/kanterae/isaconfig-dixa/downloads/isaconfig-cointoss.zip>
- b. Unzip this archive
- c. **Move the unzipped folder into the “Configurations” folder of your ISAcreeator directory (created in step1b). You should now have a path like “ISAcreeator-1.x/Configurations/isaconfig-cointoss/”**

Note: be sure to never add any files in the configuration folder, otherwise ISAcreeator will not recognize it as a valid configuration

3. ISAconfigurator

- a. Visit <http://isatab.sourceforge.net/tools.html> scroll down and click on your operating system icon under ISAconfigurator

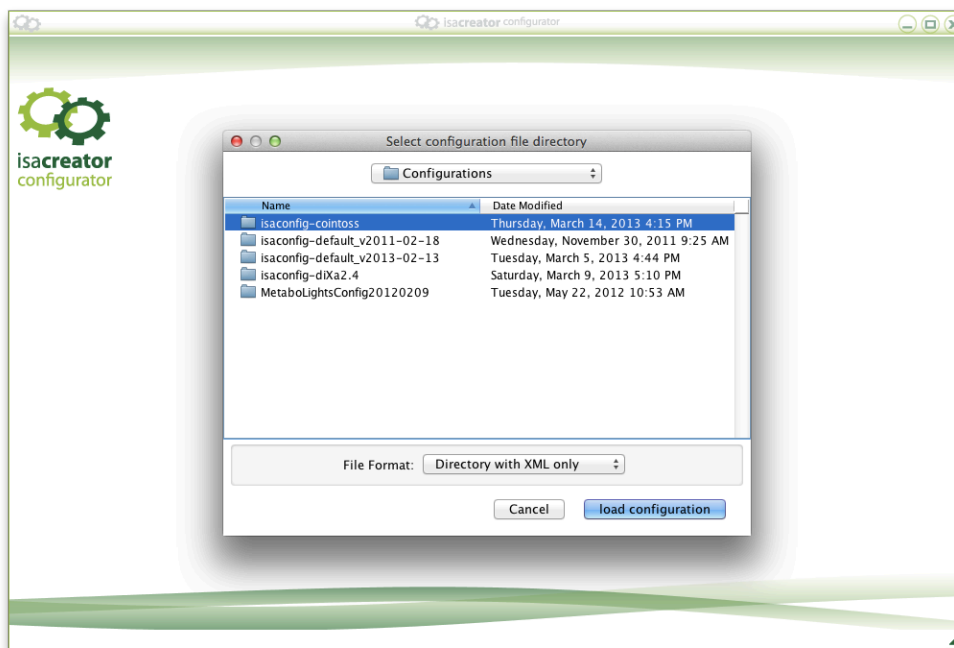


- b. Download and unzip the application

Steps

1

Start ISAconfigurator and select “Open Existing” configuration. Browse to your ISAcreeator Configurations directory and select “isaconfig-cointoss” and “load configuration”



On the left you will see 3 tables: a table for Investigation, Samples and the Coin Toss Assay. This is the standard way of structuring meta-information in ISA-tab. That is:

- **Investigation:** general information about your project or “Investigation”, such as Title, Description, Contact information and associated publications
- **Samples:** characteristics of your samples, such as Source, Material and Name
- **Assay:** parameters specific to your data collection assay, such as the protocols performed, the different labels applied and the location of the various data files associated with those protocols.

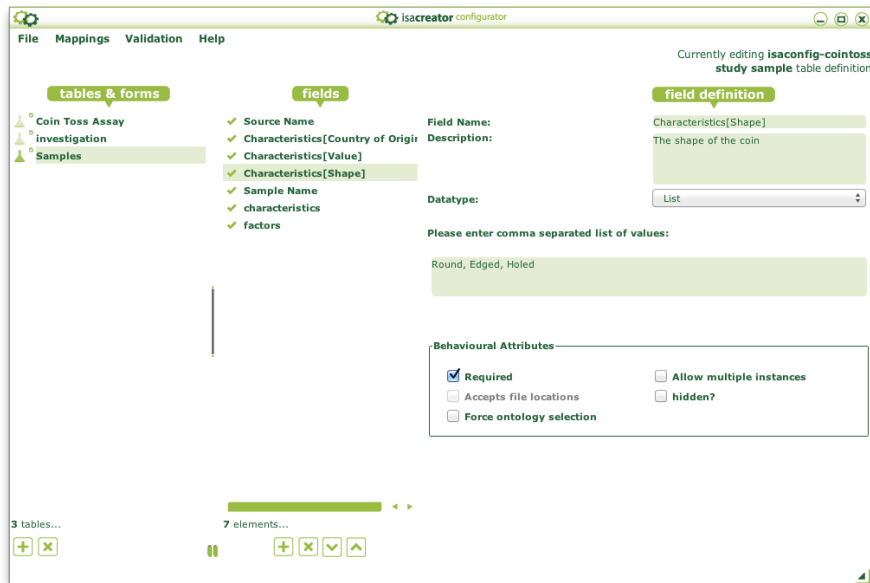
2

Click on the “Samples” table. Browse through the fields.

Source Name: Describes where the sample were obtained from

Characteristics[Country of Origin]: is an ontology field that is restricted to a list of Countries from the NCI Thesaurus ontology

Characteristics[Value]: Is a “Double” field, that is, allowing for decimal numbers. We will use this to record the value of the coin in local currency (for example 20 eurocents should be entered as 0.20)




Characteristics[Shape]: Is a list of possible coin shapes

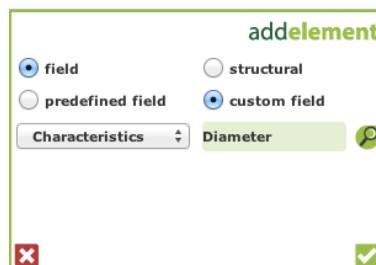
3

Add the value “**Holed**” to the list and make this a required field by checking the appropriate box.

Now let’s add an additional characteristic, the Diameter of the coin.

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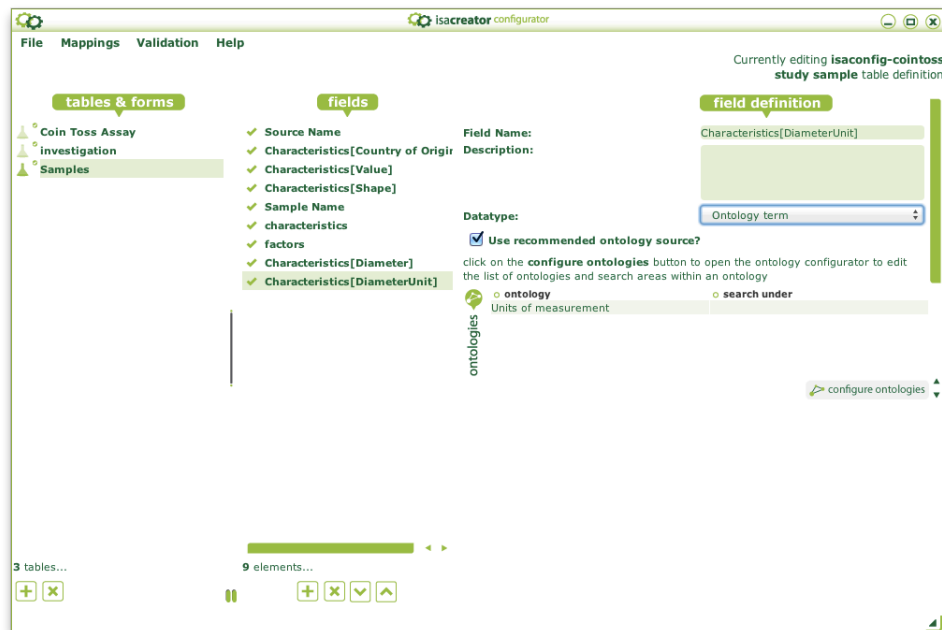
Click on  on the bottom of the fields list and select “custom field”. Then select “Characteristics” and type “**Diameter**”




Change this to be a “**Double**” field which will allow us to enter decimals

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Similarly add the following field: “**Characteristics[DiameterUnit]**” that should be an ontology term. Now try to configure a recommended ontology. Select either “Units of Measurement” or the “Units Ontology”.



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Move these two fields underneath “Characteristics[Shape]” using the up arrow  so as to conform to the ISA-tab specification

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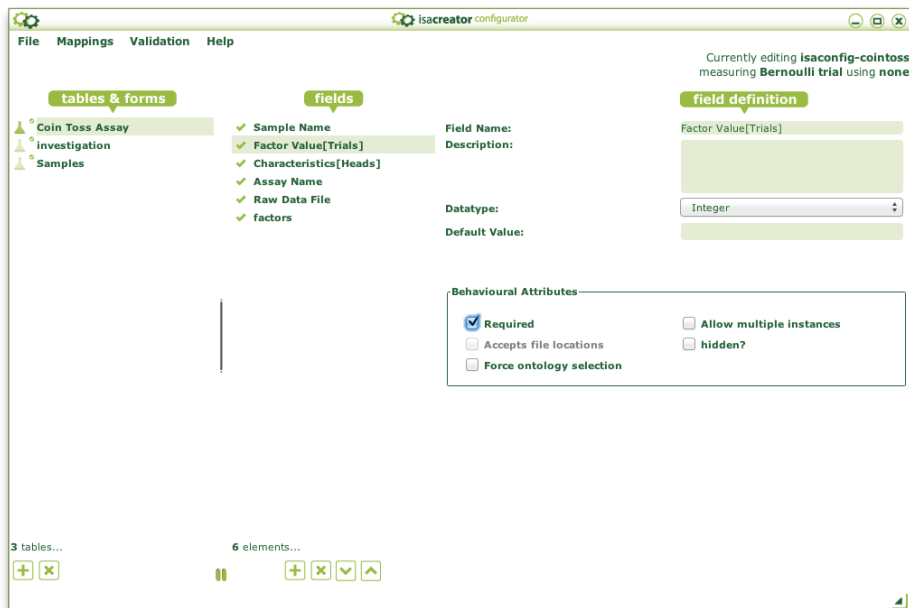
Let’s now configure the “Coin Toss Assay” table. Select it from the list on the left. Let’s add a new field. This time it will be “**Factor Value[Trials]**”

Note: “**Factor Value**” is a factor that corresponds to an independent variable manipulated by the experimentalist with the intention to affect biological systems in a way that can be measured by an assay. Whereas, “**Characteristics**”, can be any material one wishes to record about a sample or an assay.

In that sense, the number of Trials is better suited to be a “Factor Value” rather than a “Characteristic”.

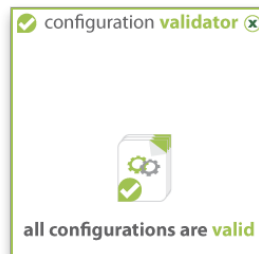
8

Set the “Factor Value[Trials]” field to be an Integer, make it a required field and move it above the “Characteristics[Heads]”

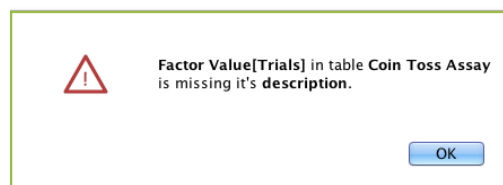


9

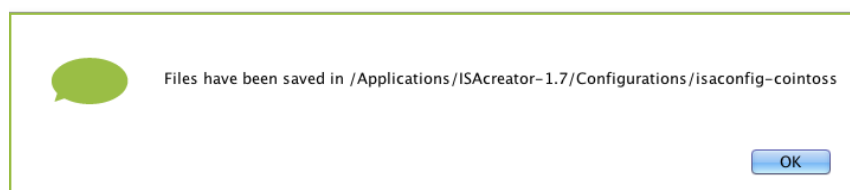
We are now finished with our configuration. Let's try to validate it. Click on Validation - Show validation errors. Seems to be all right.



Let's save our changes. Click on File – Save.



Seems that we are missing some description text. Go ahead and fill out the descriptions that are missing until you are able to save your changes.



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We'll now switch over to ISAcreeator and try to record an experiment using our configuration.

Start ISAcreeator, Select the middle start-up option and login (or create a profile if you're using ISAcreeator for the first time). Select the **"isaconfig-cointoss"** configuration we previously defined.



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Create a new experiment description – create manually

Click to add a new Study and call it the default, "Study".



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Click on “add new assay(s)”, select “+ **add assay**” (here we only have one possible assay configured. In more realistic scenarios, you may have more than one kind of assay to select from), select “Done”.

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Let’s go ahead and add some data in the “**s_Study.txt**” table. Feel free to record your own data or use the data below:

Source Name	Country of Origin	Value	Shape	Diameter	Diameter Unit	Sample Name
wallet	NCIt:United Kingdom	0.20	edged	2	UO:centimeter	Uk_20p_1
wallet	NCIt:Greece	0.01	round	1.5	UO:centimeter	Eur_1c_1

Now on the “**a_study_Bernoulli trial_none.txt**” table, enter the following:

Sample Name	Trials	Heads	Assay Name	Raw Data File
Uk_20p_1	10	4	coin toss assay	
Eur_1c_1	10	6	coin toss assay	

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Congratulations! You have successfully created an ISA-tab archive using a custom configuration. Click on File - Save, and give “**cointoss**” as the folder name.

Your study is saved by default in the same folder as the ISAcreeator executable, under the “**isatab files**” folder.

TIP: To be sure everything is in order you can validate your archive in File - Validate ISAtab.

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You can also export your ISA-tab tables as a zip archive on your Desktop. Go to File - Create ISArchive.



A file named as “**cointoss.zip**” should appear on your Desktop. This archive contains your study meta-data in ISA-tab format, as well as any data files you may have indicated, for example in the “Raw Data File” column.

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For any questions regarding this tutorial, please email training@dixa-fp7.eu with “ISAtab tutorial” in the subject header.