

Take Wing: Building Ontologies with Tawny-OWL

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Chapter 1

Introduction

This book introduces ontology building using the OWL2 ontology language, and the Tawny-OWL library. Ontologies are a method for representing knowledge, generally, but not necessarily, about the world around us. It is then possible to check that the representation is consistent, as well as drawing conclusions about new knowledge. They are generally used in complex, knowledge-rich areas of knowledge, including biomedicine.

Many ontology development tools provide a Graphical User Interface, through which the ontology developer adds the various entities involved in building an ontology. However, many ontologies contain large and repetitive sections; for these, ontology development teams often fall back to generating parts of their ontology programmatically. Tawny-OWL takes a different approach where ontology development in a domain-specific language (DSL) embedded in a full programming language. For structurally simple parts of an ontology, the various components of an ontology can be specified using the default convenient and simple Tawny-OWL syntax; for structurally complex parts, new syntax and new patterns can be built, extending the environment as a core part of ontology development.

This form of programmatic ontology development is still young. At the moment, we have used it to produce large ontologies that would have been difficult using any other technique. However, we also hope that we can also support easier integration of knowledge-rich structures into applications, so that ontological data structures can become a standard part of the programmers toolkit.

1.1 Status

This manual is a work in progress and there are quite a few bits to write yet. Once, it is somewhat more advanced, we will mark up the individual sections with status markers! This file is also available in HTML

1.2 What is an Ontology

Ontologies are about definitions. It is, perhaps, unsurprising therefore that amount ontologists there are quite a few debates about what exactly an ontology is and is not; it is not our intention here to either cover these arguments, nor to give a comprehensive overview of all the uses of the word.

What is generally agreed is that ontologies describe a set of entities, in terms of the relationships between these entities, using any of a number of different relationships. So, for example, we can describe entities in terms of their class relationships – what is true of a superclass is also true of all subclasses. Or we can describe the *partonomic* relationships: the finger is part of the hand, which is part of the foot.

An ontology is also very similar to a taxonomy; however, ontologies place much greater emphasis on their computational properties. This makes ontologies much more suitable for driving applications and code, although this often comes at the cost of human understandability of the ontology. In this document, all the ontologies we talk about are represented using specific language, called OWL (the Ontology Web Language). This has very well-defined computational properties, and through the document we will explore the implications of these properties.

We also use the term "ontology" to mean a specific object that you can manipulate in Tawny-OWL, which is a slightly more constrained use. This is quite common in many books on programming: we hope that the context should be clear.

1.3 Who this book is for

We have two primary audiences for this book. The first is for the ontologist who is interested in Tawny-OWL as the hub of a new environment for ontology development. The second is for the programmer who is interested in using the rich computational representation of a domain that ontologies provide. There is a risk to having two audiences: that we satisfy neither. To avoid this, the book is built from a series of chapters, each of which covers a

discrete topic, either more programmatic or more ontological. It should be possible to read the chapters independently of each other.

This book does not, however, stand alone. While we try to introduce the background material, we do not intend that, for example, this book will serve as an introduction to programming either in general, or specifically in Clojure. There are many good resources available for this. With ontologies, we give more of a background introduction, but again, we assume that you will be willing to read other material to clarify ontology development. Our hope is that we introduce the material well enough that you feel it is worth the time to investigate other resources, and we include pointers where it seems valuable.

Chapter 2

A Rapid Walk-Through

2.1 A Taster

We take a rapid walk-through an ontology to demonstrate the capabilities of Tawny-OWL. As with all the examples in this book, the code in this chapter is complete, therefore, we need to start with a preamble, defining a namespace and performing some imports.

```
(ns take.wing.walk-through
  (:refer-clojure :only [])
  (:use [tawny.owl]
         [tawny.english]
         [tawny.reasoner]))
```

As we discussed in Section ??, the word ontology has quite a few different meaning, but here we use it to mean a specific computational object; so, before, we do anything else, we start a new empty ontology, which we call `walk_through`; as it happens, we do not need to refer to this object again because it is now set as the default for the rest of this chapter. We also take the opportunity to set our choice of reasoner, in this case HermiT. We will see later how we use this.

```
(defontology walk_through
  :iri "http://purl.org/ontolink/walk_through")

(reasoner-factory :hermit)
```

Ontologies are all about classes, so we now define two classes one called `Book` and one called `TakeWing` which is a subclass of `Book`¹. Anything that is true of `Book` must also be true of `TakeWing`.

¹One of the joys of ontology development is that the ontology development community

```
(defclass Book)

(defclass TakeWing
  :super Book)
```

Of course, this does not tell us much about `TakeWing` as a book. There are many properties of books, but one of the most informative is the subject of the book. So, we define a new class of `Subject` and introduce a property about which we use to relate books and subjects ².

```
(defclass Subject)

(defoproperty about)
```

Now, we need some subject listings. Of course, there are many of these in existence already, and Tawny-OWL is fully capable of reusing one of these; however, for this simple example, it is not necessary, so we define a small classification of our own. We describe `Bird` and `Ontology` as subclasses of `Subject` and say that they are different (`:disjoint`) and do not overlap. We also describe `TawnyOWL` as part of the `Ontology` subject.

```
(as-subclasses
  Subject
  :disjoint
  (defclass Bird)
  (defclass Ontology))

(defclass TawnyOWL
  :super Ontology)
```

We can now make some basic queries against the statements that we have made to make sure that they all make sense. So, for example, the `subclasses` function lists all of the subclasses of `Book`, or we can use the predicate function `subclass?`. On its own this functionality is enough to build a simple hierarchy.

```
(subclasses Book)
;; => #{#[Class 0x660b9d1 "TakeWing"@en]}
```

is rich with arguments about the correct way to model things. Even, with relatively simple models it is easy to hit these arguments and, in fact, we have done so here already. There is a strong argument to say that `TakeWing` is actually an instance of `Book` rather than a subclass, because there is only one of them. Or, that `TakeWing` is a class because there are many copies of `TakeWing`. Or, that it's a metaclass, because sometimes it operates like a class and sometimes an individual. In this book, we try to touch on these arguments, but not get weighed down by them

²Strictly, an *object property*, hence the “o”. We describe these more fully later

```
(subclass? Book TakeWing)
;;=> true
(subclass? Subject TawnyOWL)
;;=> true
```

However, the functionality of OWL allows much richer statements than this. We can extend the existing definition of `TakeWing` and state that it is a book that is about `TawnyOWL` and only about `TawnyOWL`.

```
(class
  TakeWing
  :super
  (some-only about TawnyOWL))
```

Now, we can build some *defined* classes. We describe an `OntologyBook` as a `Book` which is about `Ontology`.

```
(defclass
  OntologyBook
  :equivalent
  (and Book
    (some about Ontology)))
```

There are two critical points about this definition. The first is that we had said nothing at all about the relationship between this class and `TakeWing`. We can confirm this by asking about the subclasses of `OntologyBook`, and showing that our ontology knows of no ontology books.

```
(subclasses OntologyBook)
;;=> #{}
```

However, this is not quite true. The second critical part of the definition, the use of `:equivalent`. This allows us to use *reasoning* to infer other subclasses. For this we use the `isubclasses` method instead and find that `TakeWing` can be inferred to be an `OntologyBook`.

```
(isubclasses OntologyBook)
;; => #{#[Class 0x557ef049 "TakeWing"@en]}
```

We can infer that `TakeWing` is a subclass of `OntologyBook` because we have said that an ontology book is one about ontologies and that this book is about `Tawny-OWL` which is sub-topic of ontologies. Even in this simple example, we need to put together a number of facts to draw this conclusion.

In this case, though, there is some apparent similarity between the definition of `OntologyBook` and `TakeWing` – both of them are look relatively similar, at least once we substitute `Ontology` for `TawnyOWL` in the definition of `TakeWing`. Our computational reasoner, however, does not work in this

way, and can draw conclusions even when this similarity does not exist. Consider this example where we describe books which are not about birds.

```
(defclass NonBirdBook
  :equivalent
  (and Book
    (not (some about Bird))))

(subclasses NonBirdBook)
;;=> #{}

(isubclasses NonBirdBook)
;; => #{[Class 0x557ef049 "TakeWing"@en]}
```

Here too, we can classify `TakeWing`. The chain of logic in this case is that `TakeWing` is about `Ontology`, that `Ontology` is different from `Bird`, and that, therefore, `TakeWing` is not about `Bird` which makes it a `NonBirdBook`.

This ability to infer new knowledge is the meat and drink of computational ontologies. They allow a rich description of the environment with a tightly defined semantics which makes that environment computationally accessible. Here, we have only touched on the expressivity of OWL – there are many constructs that we have not shown yet. We have also used this for only for a small ontology, but as the ontologies grow larger, the value increases.

For existing ontology developers, this will familiar ground. Tawny-OWL, however, brings something new to other mechanisms for developing ontologies; that is a fully programmatic environment. As well as the ability to automate any part of ontology development that we choose, this also brings a rich set of highly-developed tools that programmers have been developing and using for many years to develop software in a repeatable, scalable and highly-collaborative way. It is this which we explore next.

2.2 Environment

Tawny-OWL takes a different approach to other ontology development environments. It is not an application, it is just a programmatic library³. This has a key advantage over a more traditional ontology editor; rather than providing a complete environment, Tawny-OWL just recasts ontology

³Sort of. In other environments, we have argued that Tawny-OWL is an textual application rather than a programmatic library. In reality, it is a bit of both: it is a library which is designed with development rather than manipulation of ontologies as its primary purpose. For the latter, we would have done things rather differently.

development as a form of software development and borrows its entire environment from software development. This means we can reuse the software engineering environment; our experience is that the richness and maturity of software development tools far outweighs any loss of specificity to ontology development.

Our hope is that for structurally simple ontologies, Tawny-OWL should be usable by non-programmers, with a simple and straight-forward syntax. In this section, we introduce the core technology and the basic environment that is needed to make effective use of Tawny-OWL, as well as some optional extras.

2.2.1 The OWL API

Tawny-OWL is built using the <http://owlapi.sourceforge.net/> [OWL API]. This library is a comprehensive tool for generating, transforming and using OWL Ontologies. It is widely used, and is the basis for the Protege 4 editor[?]. Being based on this library, Tawny-OWL is reliable and standard-compliant (or at least as reliable and standard-compliant as Protege!). It is also easy to integrate directly with other tools written using the OWL API, include Protege.

2.2.2 Clojure

Tawny-OWL is a programmatic library build on top of the Clojure language. Tawny-OWL takes many things from Clojure. These include:

- the basic syntax with parentheses and with `:keywords`
- the ability to effectively add new syntax
- the ability to extend Tawny-OWL with patterns
- integration with other data sources
- the test environment
- the build, dependency and deployment tools

In addition, most of the tools and environment that Tawny-OWL use to enable development were built for Clojure and are used directly with little or no additions. These include:

- IDEs or editors used for writing Clojure

- the leiningen build tool

Tawny-OWL inherits a line-orientated syntax which means that it works well with tools written for any programming language; most notable among these are version control systems which enable highly collaborative working on ontologies.

Clojure is treated as a programmatic library – the user never starts or runs Clojure, and there is no `clojure` command. Rather confusingly, this role is fulfilled by Leiningen, which is the next item on the list.

2.2.3 Leiningen

<http://www.leiningen.org>[Leiningen] is a tool for working with Clojure projects. Given a directory structure, and some source code leiningen will perform many project tasks including checking, testing, releasing and deploying the project. In addition to these, it has two critical functions that every Tawny-OWL project will use: first, it manages dependencies, which means it will download both Tawny-OWL and Clojure; second, it starts a REPL which is the principle means by which the user will directly or indirectly interact with Tawny-OWL.

2.2.4 REPL

Clojure provides a REPL – Read-Eval-Print-Loop. This is the same things as a shell, or command line. For instance, we can the following into a Clojure REPL, and it will print the return value, or 2 in this case.

```
;; returns 2  
(+ 1 1)
```

The most usual way to start a REPL is to use leiningen, which then sets up the appropriate libraries for the local project. For example, `lein repl` in the source code for this document, loads a REPL with Tawny-OWL pre-loaded.

In practice, most people use the REPL indirectly through their IDE.

2.2.5 IDE or Editor

Clojure is supported by a wide variety of editors, which in turn means that they can be used for Tawny-OWL. The choice of an editor is a very personal one (I use Emacs), but in practice any good editor will work.

The editor has two main roles. Firstly, as the name suggests it provides a rich environment for writing Tawny-OWL commands. Secondly, the IDE will start and interact with a REPL for you. This allows you to add or remove new classes and other entities to an ontology interactively. Tawny-OWL has been designed to take advantage of an IDE environment; in most cases, for example, auto-completion will happen for you.

2.2.6 Testing

Tawny-OWL can use any of the testing environments that come with Clojure, including `clojure.test` which is the most basic environment provided with Clojure. This integrates well with both leiningen or an IDE both of which will run tests for you and report on test cases.

2.2.7 Version Control and Collaboration

Most ontologies are developed by many people, so some form of collaboration support is needed. In general, with Tawny-OWL we achieve this in the same way that programmers do; rather than providing a collaborative environment where multiple people can edit the environment at the same time, we use version control where different developers use slightly different versions of the ontology, and then merge them together at the end. This works well with Tawny-OWL as it has an attractive, line-orientated syntax. The various version control tools can scale easily to thousands of developers which is well in excess of most ontology projects. For this purpose, we use `git`.

2.2.8 Continuous Integration

An ontology can be *continuously integrated* with both other ontologies that it depends on, and with the software environment which uses it. Unlike other ontology continuous integration systems, Tawny-OWL is just a library – so anything that works with Clojure (or more abstractly a Java Virtual Machine) will also work with Tawny-OWL.

2.3 Recap

In this Chapter, we have built a small basic ontology which non-the-less shows the computational power of OWL ontologies, while surveying the

advantages that Tawny-OWL brings as a development environment for ontologies.

Chapter 3

An Introduction to OWL

In Section 1.2, we briefly touched on the issue of what is an ontology and noted that it's not easy. In this section, we will take a more pragmatic view point and describe OWL and its notion of an ontology.

OWL2 is the second version of the Ontology Web Language; it is a W3C recommendation¹. As you might expect, this means that it embeds well with other W3C standards – it can be serialized as XML or RDF, and it makes quite intensive use of URLs.

It also builds on many years of Computing research; underneath each of the statements that we can make in OWL is a mapping to a piece of formal maths which gives a tightly defined *semantics*. We will only touch of this semantics lightly in this document²; the key point is that this specification makes it possible to build software around OWL and have it come to a clearly defined conclusions.

Using the statements in OWL we can build models of the world. That is we can describe the real world around us using statements in OWL; as a result, we can use these underlying semantics of OWL to draw conclusions about these models. If we do this right, these conclusions should also be true of the real world as well.

There are a number of different ways that we could build models, but OWL does this with three entities: individuals, classes and properties. In addition, to enable OWL ontologies to describe the real world, it also has two further entities: identifiers and annotations.

¹W3C is the body that would define standards for the Web, if it makes standards. Except that it does not; it just releases recommendations.

²Mostly because if I touched on it more heavily, I'd probably get it wrong

3.1 Individuals

At heart, OWL ontologies describe a set of individuals. In the real world, these would be the things that we want to describe. Looking around me now, I can see a large number of these things: a computer screen (obviously); a keyboard; assorted other pieces of computing detritus; a guitar; a door; and, finally, somewhat incongruously, a toilet seat. Individuals in OWL can also describe more abstract things such as the image on my screen, the process of me typing and so forth.

Sometimes, individuals are also called instances; we do not use this term here, because it causes confusion with people who come Object-Oriented programming background where it has a related but subtly different meaning³.

In OWL ontologies, individuals also have a name or an identifier⁴. Actually, they can any number of names and, perhaps, unintuitively, OWL will not assume that they have an unique name; so, unless you tell it explicitly, OWL will not know whether two different identifiers describe two different individuals with one name each, or one individual with two names.

3.2 Properties

Individuals can have relations between them. In OWL, these are called properties⁵. So, the `I` and `typing` on my `Keyboard`. In OWL properties are *binary* – that is they only describe a relationship between two individuals⁶. Properties in OWL have a number of characteristics, which we will describe later.

It is also possible to use properties to describe a relationship between an individual and something *concrete* – such as a numeric value or a string.

3.3 Classes

Classes in OWL are *sets* on individuals. All the individuals in a class will share some of the same characteristics. Classes have relationships between themselves which turn them into a hierarchy. So, both my `Trackball`,

³Like “object” which also has an ontological meaning.

⁴Although, some individuals are anonymous. We will discuss more on the form of identifiers later.

⁵Roughly equivalent to properties or attributes in OO terminology

⁶This is less restrictive than it sounds.

`Keyboard` and `Monitor` are subclasses of `Peripherals`. In OWL, the meaning of the subclass relationship is quite specific – if `A` is a subclass of `B`, then all individuals of class `A` are also individuals of class `B`.

For people coming from an programming background, this looks very like object-orientation (OO) and its notion of instances, classes and subclasses. But there is subtle, but important difference. In OO, instances are explicitly stated to be part of a class, and inherit properties from this class. In OWL, it is the other way around: individuals have properties, and then properties that they have define the classes that they are in. We can see this in Section 2.1, where we can *infer* that `TakeWing` is an `OntologyBook`.

3.4 Identifiers

To make all of the logical entities in OWL useful, we need *identifiers* which allows us to refer to them. Again, most programming languages have this sort of capability: variable names, class names and so forth. OWL is rather different here and shows its web heritage; it uses IRIs for identifiers⁷.

Identifiers in OWL, therefore, are effectively universal; a class in one ontology can unambiguously refer to a class in another. More over, it can use and share identifiers described and defined in all the other web technologies.

Tawny-OWL maps these identifiers on to its own which inherits from its base language of Clojure; this largely stems from the requirements for identifiers which are easy to type and use.

3.5 Annotations

Those who are interested in the underlying semantics of OWL often describe annotations are *extra-logically*. This rather downgrades their importance; it is annotations that allow the underlying logic to relate to the real world around. The underlying logic of OWL may provides predictable behaviour, but is the annotations which provide all the utility of an OWL ontology, by relating to the real world and to the user.

OWL allows annotations on pretty much anything. Classes, individuals and properties can all have annotations; the axioms that assert these entities can have annotations; annotations can have annotations; it is even possible to use annotations to provide descriptions of why annotations have annotations. It is entirely possible that the designers of OWL got a little carried

⁷IRIs are not the same thing as URIs, which are not the same thing as URLs. But the differences between them are relative unimportant here.

away with annotations, Tawny-OWL supports the many different forms of annotation anyway.

Chapter 4

Getting Started

In this section, we will build the most ontology and start to show the basic capabilities of Tawny-OWL.

As described in , Tawny-OWL can be used with several different toolchains. In this section, we will run through the building a very simple ontology. There is an section describing how to achieve each of these steps with specific tool chains.

4.0.1 Installing Leiningen

To build an ontology, we need a build tool, for which we will use <https://leiningen.org>leiningen. This is a command line application and is simple to install following the instructions on their website.

Installing leiningen is the only manual step involved. It is leiningen that is responsible for everything else; it downloads Tawny-OWL and all of its dependencies for you.

4.0.2 Creating a New Project

Now, we will create a new project. Tawny-OWL makes this easy with a pre-defined template.

```
lein new ontology helloworld
```

This will create a new directory called `helloworld`. If we change into this directory, we find that this has created a number of directories and files.

Before we look in more detail at these files, let start by generating an ontology file. Simply type:

```
lein run
```

You should see that a new file has been created called `helloworld.omn` which contains a very simple ontology with a single class called `HelloWorld`.

4.0.3 Editing Our Ontology

Tawny-OWL provides a fully programmatic development environment for ontologies; as such, it is possible to change or update an ontology with an editor or any IDE. In this section, we will use a simple, web-based editor that integrates tightly with leiningen.

To use this try:

```
lein with-profile light nightlight
```

This should return something like:

```
Started Nightlight on http://localhost:4000
```

Open this address in a web-browser and you should now be able to see the editor. This in turn will enable you to look at the Tawny-OWL files.

First, we consider the file `helloworld.clj`; this looks like so:

```
(ns helloworld.helloworld
  (:use [tawny.owl]))

(defontology helloworld
  :iri "http://example.com/helloworld")

(defclass HelloWorld)
```

Breaking this down. We first start with by introducing the namespace and `using` Tawny-OWL. These identical statements appear at the beginning of every Tawny-OWL file: the namespace introduced must match the file name.

Next, we create a new ontology called `helloworld`, with a single class also called (somewhat repetitively), `HelloWorld`. Tawny-OWL is case-sensitive, so these two things are independent from each other.

The second file, `core.clj` is more programmatic in nature. It `requires` `helloworld`, and then defines a function called `-main` which saves the ontology.

```
(ns helloworld.core
  [:use [tawny.owl]]
  [:require [helloworld.helloworld]])

(defn -main [& args]
  (save-ontology helloworld.helloworld/helloworld "helloworld.omn"))
```

The practical upshot of this all taken together is that typing

```
lein run
```

at the command line will result in a new file (called `helloworld.omn`) with an ontology in OWL Manchester Notation (OMN).

4.0.4 Summary

In this section, we have outlined the basic tasks that are needed to build ontologies with Tawny-OWL: creating a project, creating an ontology, creating some entities. We have also started to show how to use and query over them. In the next section, we will build this ontology in full, using it to demonstrate many parts of Tawny-OWL and OWL ontologies in general.

Chapter 5

The Pizza Ontology

5.1 Introduction

In this section, we will create a Pizza ontology; we choose pizzas because they are simple, well-understood and compositional (see here for more).

As we described in a previous Chapter 3, we consider the different types of entities present in an OWL ontology. The most (and least!) important of these are *individuals*. We say that these are the most important because it is these individuals that are described and constrained by the other objects. We say that they are the least important because, in practice, many ontologies do not explicitly describe any individuals at all.

If this seems perverse, consider a menu in a pizza shop. We might see an item saying "Margherita...5.50". The menu makes no statements at all about an individual pizza. It is saying that any margherita pizza produced in this restaurant is going to (or already has) cost 5.50. From the menu, we have no idea how many margherita pizzas have been produced or have been consumed. But, menu is still useful. The menu is comprehensive, tells you something about all the pizzas that exist (at least in one restaurant) and the different types of pizza. This is different to the bill, which describes individuals – the pizzas that have actually been provided, how many pizza and how much they all cost. In ontological terms, the menu describes the **classes**, the bill describes individuals ¹. OWL Ontologies built with Tawny-OWL *can* describe either or both of these entities but in most cases focus on classes.

¹The analogy between a pizza menu and an ontology is not perfect. With pizza, people are generally happy with the classes (i.e. the menu) and start arguing once about the individuals (i.e. the bill); with ontologies it tends to be the other way around

5.2 Creating the Skeleton

As we discussed in Section 4.0.2, it is possible to use `lein` to create a new ontology project. We will do this now:

```
lein new ontology take-wing-pizza
```

This will create a directory called `take-wing-pizza`². We can now edit the files in this directory, starting with `take/wing/pizza.clj` using either `nightlight` as described in Section 4.0.3, or any other IDE.

5.3 Preamble

In Chapter 2, we showed the standard template for a Tawny-OWL file; and indeed, `lein` has created a pizza themed version for us.

```
(ns take.wing.pizza
  (:require [tawny.owl :refer :all]))
```

It is not absolutely critical to understand these statements, but they are simple enough and worth explaining now, even though they will become much more relevant and start to exploit the underlying programming language of Tawny-OWL, that is Clojure.

Statements in Clojure are also known as “forms”. Pretty much all Clojure forms have the same structure; that is they are delimited by `(` and `)`. Forms are usually named after the first letters that appear in them, which is the name of the function they will call; so in this case, we have a `ns` or “namespace” form. Forms can be nested. The `:require` form is an example of this. In this case, the `:require` says simply to make the Tawny-OWL functions available for use. The colon in `:require` means that this is a *keyword*. Tawny-OWL uses these in many places to define parameters, as we see next. Before we go any further, let’s make this slightly more complex:

```
(ns take.wing.pizza
  (:require [tawny.owl :refer :all]
            [tawny.reasoner :as r]))
```

We will see the importance of `tawny.reasoner` later. Next, we have a `defontology` form which looks like this:

```
(defontology take-wing-pizza
  :iri "http://example.com/take-wing-pizza")
```

²The name of this directory is not functional important and be changed at will

The name of the function `defontology` tells us something useful; as well as creating an ontology, we are defining a name which we can use to refer to the ontology. The name is `take-wing-pizza` which comes next. Finally, we define some parameters – in this case, the IRI. All OWL ontologies require IRIs (strictly the Ontology IRI) by which they can be referred³. Here, we invent one in the `example.com` domain. You should change this to an IRI you control. In this case, we use one from `purl.org`.

```
(defontology take-wing-pizza
  :iri "http://purl.org/ontolink/take-wing/pizza")
```

The semantics of this statement are quite interesting. If we had created a new database, by default, the database would be considered to be empty – that is there would be no individuals in it. With an ontology, the opposite is true. By default, we assume that there could be any number of individuals. As of yet, we just have not said anything about these individuals.

5.4 Defining Classes

Next, we declare two classes. A class is a set of individuals with shared characteristics. The basic template creates an entirely useless `HelloWorld` task for us like so:

```
(defclass HelloWorld)
```

This follows the same syntax as all forms with (and), and follows the convention of `defontology` – a class object is created as well as a name `HelloWorld` which we can use to refer to that object. In this case, we do not add any arguments nor do we need to. If you are using `nightlight`, it should look like this:

It is possible to run, or evaluate, Tawny-OWL files as well. To see this in `nightlight`, simply select “Insta-REPL” on the top-right.

On the left, we can see the results of this evaluation. The actual values are not that useful in Tawny-OWL, but the that they are green shows that they are valid.

Clearly, as this is supposed to be an ontology of pizza rather than classic computer programs, we will need to change this. So, first we replace `HelloWorld` with `Pizza` and add a new class called `PizzaComponent`. As with our `defontology` form, have a `def` form; however, in this case, we do not use

³In Tawny-OWL, this requirement is weakened – if you do not put an IRI, Tawny-OWL invents one for you. This is okay if you are experiments, but should be changed when you publish an ontology.

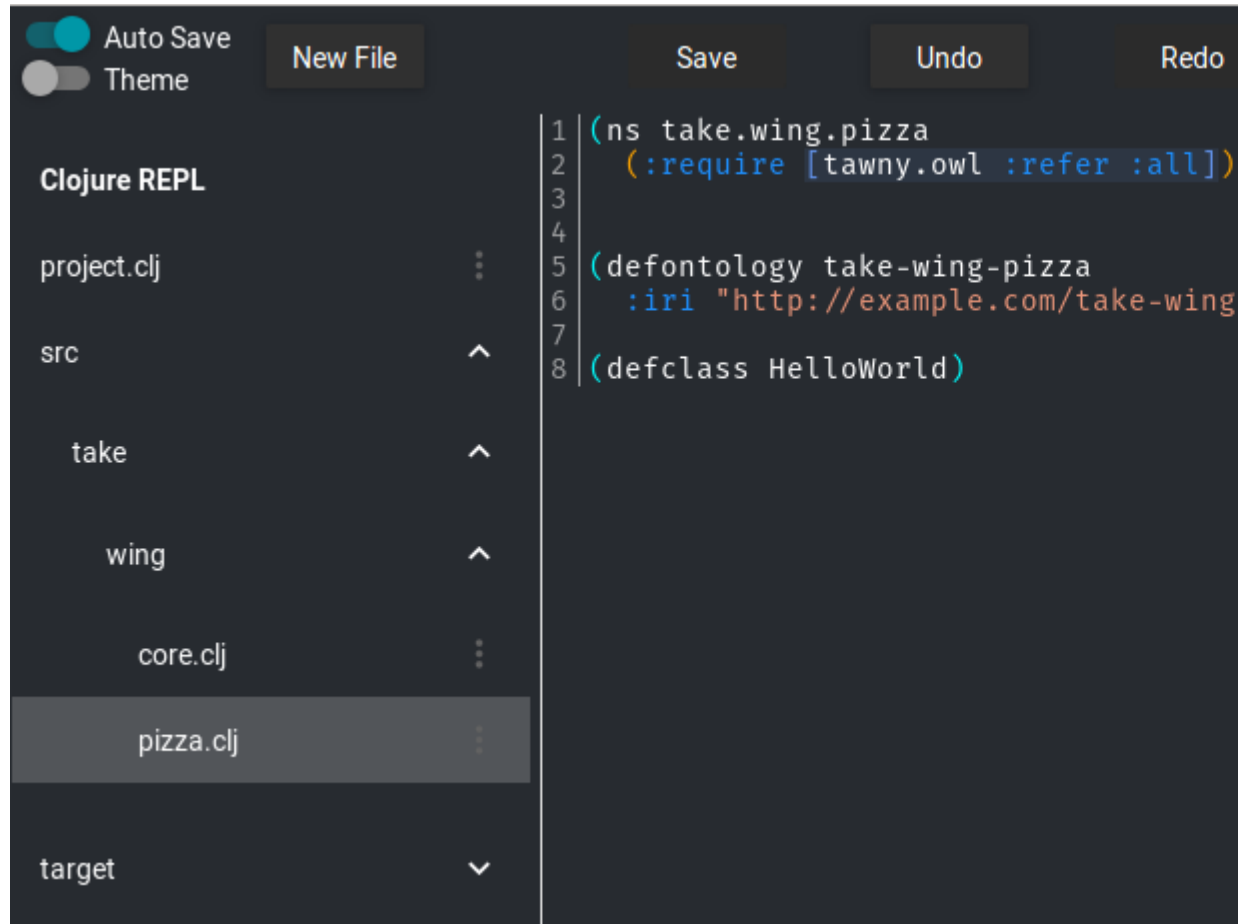


Figure 5.1: A new pizza ontology

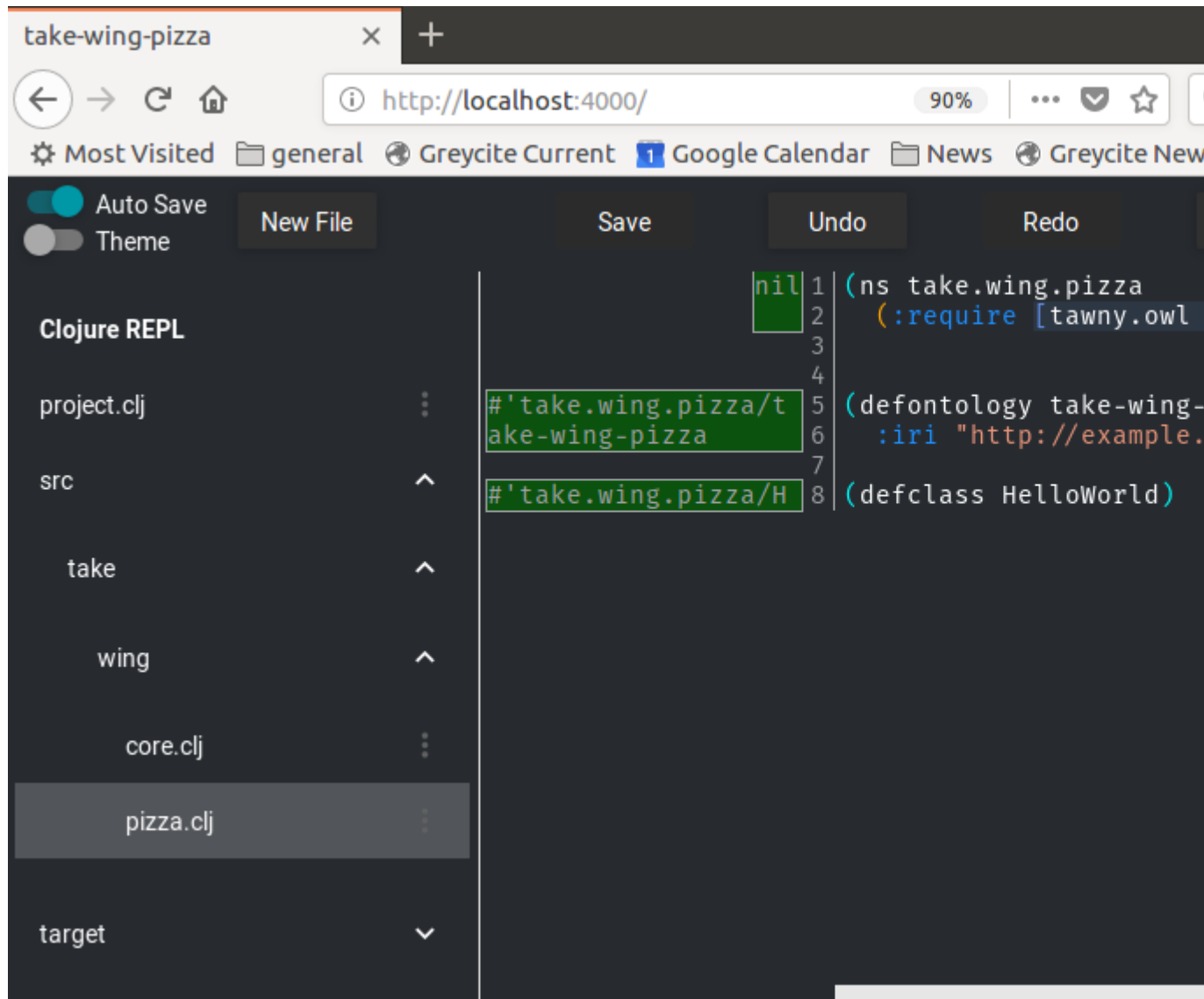


Figure 5.2: The Insta-REPL

any arguments. The semantics of these two statements are that, there is a class called `Pizza` and another called `PizzaComponent` which individuals may be members of. However, we know nothing at all about the relationship between an individual `Pizza` and an individual `PizzaComponent`⁴.

```
(defclass Pizza)
(defclass PizzaComponent)
```

To build an accurate ontology, we may wish to describe this relationship further. We might ask the question, can an individual be both a `Pizza` and a `PizzaComponent` at the same time. The answer to this is no, but currently our ontology does not state this. In OWL terminology, we wish to say that these two classes are *disjoint*. We can achieve this by adding an `as-disjoint` statement.

```
(as-disjoint Pizza PizzaComponent)
```

This works well, but is a little duplicative. If we add a new class which we wish to also be disjoint, it must be added in two places. Instead, it is possible to do both at once. This has the advantage of grouping the two classes together in the file, as well as semantically, which should make the source more future-proof; should we need new classes, we will automatically become disjoint as required.

```
(as-disjoint
 (defclass Pizza)
 (defclass PizzaComponent))
```

If you are using Nightlight, you may find it a little hard to edit your file to achieve this as Nightlight uses `parinfer`. This puts the parentheses in place for you. To make this statement, type `as-disjoint` before the other two forms:

```
(as-disjoint)
(defclass Pizza)
(defclass PizzaComponent)
```

Now, add two spaces in front of `defclass Pizza`) and then `(defclass PizzaComponent)`. The parentheses should take care of themselves.

```
(as-disjoint
 (defclass Pizza
```

⁴In this ontology, we use a naming scheme using CamelCase, upper case names for classes and, later, lower case properties. As with many parts of ontology development, opinions differ as to whether this is good. With Tawny-OWL it has the fortuitous advantage that its syntax highlights nicely, because it looks like Java class names.

```

:label "Pizza"
:comment "A type of prepared food, originating from Italy, consisting of a
flatbread with any of a large variety of other foods on top."
(defclass PizzaComponent
  :label "Pizza Component"
  :comment "Food that is part of a pizza."))

```

The semantics of these statements are that our ontology may have any number of individuals, some of which may be `Pizza`, some of which may be `PizzaComponent`, but none of which can be both `Pizza` and `PizzaComponent` at the same time. Before we added the `as-disjoints` statement, we would have assumed that it was possible to be both. We also add to this two *annotations* that can be used to provide more contextualized information about the pizza – in this case a label and a comment.

As well as describing that two classes are different, we may also wish to describe that they are closely related, or that they are *subclasses*. Where one class is a subclass of another, we are saying that everything that is true of the superclass is also true of the subclass. Or, in terms of individuals, that every individual of the subclass is also an individual of the superclass.

Next, we add two more classes, in this case classes for base and toppings. We include the statement that they have `PizzaComponent` as a superclass. We do this by adding a `:super` argument or *frame* to our `defclass` statement.

```

(defclass PizzaBase
  :super PizzaComponent)
(defclass PizzaTopping
  :super PizzaComponent)

```

In Tawny-OWL, the frames can all be read in the same way. Read forwards, we can say `PizzaBase` has a superclass `PizzaComponent`, or backwards `PizzaComponent` is a superclass of `PizzaBase`. Earlier, we say the `:iri` frame for `defontology` which is read similarly – pizza has the given IRI.

As every individual of, for example, `PizzaBase` is `PizzaComponent`, and no `PizzaComponent` individual can also be a `Pizza` this also implies that no `PizzaBase` is a `Pizza`. In otherwords, the disjointness is inherited.

As with the disjoint statement, this is little long winded; we have to name the `PizzaComponent` superclass twice. Tawny-OWL provides a short cut for this, with the `as-subclasses` function.

```

(as-subclasses
  PizzaComponent
  (defclass PizzaBase)
  (defclass PizzaTopping))

```

We are still not complete; we asked the question previously, can you be both a `Pizza` and a `PizzaComponent`, to which the answer is no. We can apply the same question, and get the same answer to a `PizzaBase` and `PizzaTopping`. These two, therefore, should also be disjoint. However, we can make a stronger statement still. The only kind of `PizzaComponent` that there are either a `PizzaBase` or a `PizzaTopping`. We say that the `PizzaComponent` class is *covered* by its two subclasses⁵. We can add both of these statements to the ontology also.

```
(as-subclasses
  PizzaComponent
  :disjoint :cover
  (defclass PizzaBase)
  (defclass PizzaTopping))
```

We now have the basic classes that we need to describe a pizza.

5.5 Properties

Now, we wish to describe more about `Pizza`; in particular, we want to say more about the relationship between `Pizza` and two `PizzaComponent` classes. OWL provides a rich mechanism for describing relationships between individuals and, in turn, how individuals of classes are related to each other. As well as there being many different types of individuals, there can be many different types of relationships. It is the relationships to other classes or individuals that allow us to describe classes, and it is for this reason that the different types of relationships are called *properties*.

A `Pizza` is built from one or more `PizzaComponent` individuals; we first define two properties⁶ to relate these two together, which we call `hasComponent` and `isComponentOf`. The semantics of this statement is to say that we now have two properties that we can use between individuals.

As with classes, there is more that we can say about these properties. In this case, the properties are natural opposites or inverses of each other. The semantics of this statement is that for an individual `i` which `hasComponent` `j`, we can say that `j` `isComponentOf` `i` also.

```
(as-inverse
```

⁵For those from an OWL background, you may have noticed that “covering” is not part of the OWL standard; in fact, it’s a pattern that is frequently used. The semantics are that `PizzaComponent` is equivalent to `PizzaBase` or `PizzaTopping`

⁶Actually, two *object* properties, hence *defobjectproperty*. We can also define *data* properties, which we will see later


```
(defoproperty hasComponent)
(defoproperty isComponentOf))
```

The semantics here are actually between individuals, rather than classes. This has an important consequence with the inverses. We might make the statement that `Pizza hasComponent PizzaComponent`, but this does not allow us to infer that `PizzaComponent isComponentOf Pizza`. The way that we have named our classes for pizzas, this might be unintuitive. Consider bikes instead: just because all bicycles have wheels, we can not assume that all wheels are parts of a bike; we **can** assume that where a bike has a wheel, that wheel is part of a bike. This form of semantics is quite subtle, and is an example of where statements made in OWL are saying less than most people would assume ⁷.

We now move on to describe the relationships between `Pizza` and both of `PizzaBase` and `PizzaTopping`. For this, we will introduce three new parts of OWL: subproperties, domain and range constraints and property characteristics, which we define in Tawny-OWL as follows:

```
(defoproperty hasTopping
  :super hasComponent
  :range PizzaTopping
  :domain Pizza)

(defoproperty hasBase
  :super hasComponent
  :characteristic :functional
  :range PizzaBase
  :domain Pizza)
```

First, we consider sub-properties, which are fairly analogous to sub-classes. For example, if two individuals `i` and `j` are related so that `i hasTopping j`, then it is also true that `i hasComponent j`.

Domain and range constraints describe the kind of entity that be at either end of the property. So, for example, considering `hasTopping`, we say that the domain is `Pizza`, so only instances of `Pizza` can have a topping, while the range is `PizzaTopping` so only instances of `PizzaTopping` can be a topping.

Finally, we introduce a *characteristic*. OWL has quite a few different characteristics which will introduce over time; in this case *functional* means means that there can be only one of these, so an individual has only a single

⁷We will see examples of the opposite also — statements which are stronger in OWL than the intuitive interpretation

base. We do not make the same statement about toppings, so by default, OWL will assume that you can have any number of toppings on a pizza.

5.6 Populating the Ontology

We now have enough expressivity to describe quite a lot about pizzas. So, we can now set about creating a larger set of toppings for our pizzas. First, we describe some top level categories of types of topping. As before, we use `as-subclasses` function and state further that all of these classes are disjoint. Here, we have not used the `:cover` option. This is deliberate, because we cannot be sure that these classes describe all of the different toppings we might have; there might be toppings which fall into none of these categories⁸.

```
(as-subclasses
 PizzaTopping
 :disjoint
 (defclass CheeseTopping)
 (defclass FishTopping)
 (defclass FruitTopping)
 (defclass HerbSpiceTopping)
 (defclass MeatTopping)
 (defclass NutTopping)
 (defclass SauceTopping)
 (defclass VegetableTopping))
```

When defining a large number of classes at once, Tawny-OWL also offers a shortcut, which is `declare-classes`. While this can be useful in a few specific circumstances, these are quite limited because it does not allow addition of any other attributes at the same time, and in particular labels which most classes will need. It is quite useful in tutorial document.

```
(as-subclasses
 CheeseTopping
 :disjoint

 (declare-classes
  GoatsCheeseTopping
  GorgonzolaTopping
  MozzarellaTopping
  ParmesanTopping))
```

⁸For example, we leave open the option of a pizza base with nutella on it; it's not clear whether this is a pizza or not, but if we did decide one way or another, it would be possible to describe this clearly and explicitly in OWL.

A similar, if slightly longer-winded, way of defining many classes at once is `defclassn`. We use this to define vegetables.

```
(as-subclasses
  VegetableTopping
  :disjoint

  (defclassn
    [PepperTopping
     :label "Pepper Topping"]
    [GarlicTopping
     :label "Garlic Topping"]
    [PetitPoisTopping]
    [AsparagusTopping]
    [TomatoTopping]
    [ChilliPepperTopping]))
```

We add classes describing meat.

```
(as-subclasses
  MeatTopping
  :disjoint
  (defclass HamTopping)
  (defclass PepperoniTopping))
```

And, finally, fruit.

```
(as-subclasses
  FruitTopping
  (defclass PineappleTopping))
```

In this case, we have only a single entity, that is `PineappleTopping`, so we have not made this disjoint. In fact, Tawny-OWL would treat this as an error, since having a single disjoint class does not really make sense, and it is mostly likely it is wrong. This does mean that we need to remember to add this `:disjoint` statement, if another `FruitTopping` is added.

5.7 Describing a Pizza

And, now finally, we have the basic concepts that we need to build a pizza. First, we start off with a generic description of a pizza; we have already defined the class above, so we want to extend the definition rather than create a new one. We can achieve this using the `class` function:

```
(owl-class Pizza
  :super
```

```
(owl-some hasTopping PizzaTopping)
(owl-some hasBase PizzaBase))
```

This introduces several new features of Tawny-OWL:

- this use of `class` requires that `Pizza` already be defined. In other words, we are extending an existing definition. If `Pizza` is not defined, this form will crash.
- a new function `some`
- we create out first *unnamed* classes from a class expression – in this case `(owl-some hasTopping PizzaTopping)`.

The semantics of the last two of these are a little complex. Like a named class (all of those we have seen up to now), an unnamed class defines a set of individuals, but it does so by combining other parts of the ontology. The `owl-some` restriction describes a class of individuals with at least one relationship of a particular type. So `(owl-some hasTopping PizzaTopping)` describes the set of all individuals related by the `hasTopping` relationship to at least one `PizzaTopping`. Or alternatively, each `Pizza` must have a `PizzaTopping`. Or, alternatively again, for each `Pizza` there must exist one `PizzaTopping`; it is for this reason that this form of class is also known as an *existential restriction*.

We combine the two statements to say that a `Pizza` must have at least one base and at least one topping. Actually, we earlier defined `hasBase` with the `:functional` characteristic, so together this says that a `Pizza` must have exactly one base.

Finally, we can build a specific pizza, and we start with one of the simplest pizza, that is the margherita. This has two toppings, mozzarella and tomato. The definition for this is as follows:

```
(defclass MargheritaPizza
  :super
  Pizza
  (owl-some hasTopping MozzarellaTopping)
  (owl-some hasTopping TomatoTopping)
  (only hasTopping (owl-or MozzarellaTopping TomatoTopping)))
```

The first part of this definition is similar to `Pizza`. It says that a `MargheritaPizza` is a `Pizza` with two toppings, mozzarella and tomato. The second part of the definition adds two new features of Tawny-OWL:

- only a new function which returns a *universal restriction*

- `owl-or` which returns a *union restriction*

The `owl-or` statement defines the set of individuals that is either `MozzarellaTopping` or `TomatoTopping`. The only statement defines the set of individuals whose toppings are either `MozzarellaTopping` or `TomatoTopping`. One important thing in the tail of `only` is that it does **NOT** state that these individuals have any toppings at all. So `(only hasTopping MozzarellaTopping)` would cover a `Pizza` with only `MozzarellaTopping`, but also many other things, including things which are not `Pizza` at all. Logically, this makes sense, but it is counter-intuitive ⁹.

For completeness, we also define `HawaiianPizza` ¹⁰.

```
(defclass HawaiianPizza
  :super
  Pizza
  (owl-some hasTopping MozzarellaTopping)
  (owl-some hasTopping TomatoTopping)
  (owl-some hasTopping HamTopping)
  (owl-some hasTopping PineappleTopping)
  (only hasTopping
    (owl-or MozzarellaTopping TomatoTopping HamTopping PineappleTopping)))
```

We can now check that this works as expected by using the `subclass?` and `subclasses` functions at the REPL.

```
take.wing.pizza> (subclass? Pizza MargheritaPizza)
true
take.wing.pizza> (subclasses Pizza)
#{#[Class 0x74c8b756 "HawaiianPizza"@en] #[Class 0x4f1495bd "MargheritaPizza"@en]}
```

5.8 A simple pattern

The last definition is rather unsatisfying for two reasons. Firstly, the multiple uses of `(owl-some hasTopping)` and secondly because the toppings are duplicated between the universal and existential restrictions. Two features of Tawny-OWL enable us to work around these problems.

Firstly, the `owl-some` function has a special property – it *broadcasts*. This means it can take a single property but any number of classes; this is

⁹Except to logicians, obviously, to whom it all makes perfect sense.

¹⁰Pizza names are, sadly, not standardized between countries or restaurants, so I've picked on which is quite widely known. Apologies to any Italian readers for this and any other culinary disasters which this book implies really are pizza.

equivalent to multiple calls to the `owl-some` with a single class. We use this feature to shorten the definition of `AmericanPizza`.

```
(defclass AmericanPizza
  :super
  Pizza
  (owl-some hasTopping MozzarellaTopping
            TomatoTopping PepperoniTopping)
  (only hasTopping (owl-or MozzarellaTopping TomatoTopping PepperoniTopping)))
```

The single `owl-some` function call here expands to three existential restrictions, each of which becomes a super class of `AmericanPizza` – mirroring the definition of `HawaiianPizza`.

This definition, however, still leaves the duplication between the two sets of restrictions. This pattern is frequent enough that Tawny-OWL provides special support for it in the form of the `some-only` function, which we use to define the next pizza.

```
(defclass AmericanHotPizza
  :super
  Pizza
  (some-only hasTopping MozzarellaTopping TomatoTopping
            PepperoniTopping ChilliPepperTopping))
```

The `some-only` function is Tawny-OWL’s implementation of the *closure* axiom. Similarly, the use of `:cover` described earlier implements the *covering* axiom. These are the only two patterns which are directly supported by the core of Tawny-OWL (i.e. the namespace `tawny.owl`). In later sections, though, we will see how to exploit the programmatic nature of Tawny-OWL to build arbitrary new patterns for yourself.

5.9 Defined Classes

So far all of the classes that we have written are *primitive*. This is not a statement about their complexity. It means that as they stand, they cannot be used to infer new facts. So, for example, we know that a individual `MargheritaPizza` will have a `MozzarellaTopping` and a `TomatoTopping`, but given an arbitrary pizza we cannot determine whether it is a `margherita`. Or, `mozzarella` and `tomato` toppings are *necessary* for a `margherita`, but they are not sufficient.

Defined classes allow us to take advantage of the power of computational reasoning. Let us try a simple example:

```
(defclass VegetarianPizza
```

```

:equivalent
(owl-and Pizza
  (only hasTopping
    (owl-not (owl-or MeatTopping FishTopping)))))

```

Here, we define a `VegetarianPizza` as a `Pizza` with only `MeatTopping` or `FishTopping`. The two key point about this definition is that we have marked it as `:equivalent` rather than `:super` and that there is no stated relationship between `VegetarianPizza` and `MargheritaPizza`. We can confirm this at the shell.

```

(subclasses VegetarianPizza)
=> #{}
(subclass? VegetarianPizza MargheritaPizza)
=> false

```

However, now let us ask the same question of a reasoner. You may remember that earlier we added `tawny.reasoner` to our namespace form. This now allows us to perform computational reasoning. First, we choose a reasoner to use (in this case `HermiT`); we do this by calling the `reasoner-factory` function; this is in the `tawny.reasoner` namespace, which we can call by the short-cut name `r`.

```

(r/reasoner-factory :hermit)
=> #object[org.semanticweb.HermiT.Reasoner$ReasonerFactory 0x7d56d721 "org.semanticweb.Hermit"]

```

Then ask the same questions of Tawny-OWL but now using the versions of functions prefixed with an `i` (for inferred).

```

(r/isubclasses VegetarianPizza)
=> #{#[Class 0x6487d60d "MargheritaPizza"@en]}
(r/isubclass? VegetarianPizza MargheritaPizza)
=> true

```

Now, we see a different result. A `MargheritaPizza` is a subclass of `VegetarianPizza`, even those we have never stated this explicitly. The reasoner can infer this using the following chain of logic:

- `MargheritaPizza` has only `MozzarellaTopping` or `TomatoTopping`
- `MozzarellaTopping` is a `CheeseTopping`
- `TomatoTopping` is a `VegetableTopping`

- `CheeseTopping` is disjoint from `MeatTopping` and `FishTopping`
- Likewise, `TomatoTopping` is not a `MeatTopping` or `FishTopping`
- Therefore, `MargheritaPizza` has only toppings which are not `MeatTopping` or `FishTopping`.
- A `VegetarianPizza` is any `Pizza` which has only toppings which are not `MeatTopping` or `FishTopping`.
- So, a `MargheritaPizza` is a `VegetarianPizza`.

Even for this example, the chain of logic that we need to draw our inference is quite long. The version of the pizza ontology presented here is quite small, so while we can follow and reproduce this inference easily by hand. For a larger ontology it would be a lot harder, especially, when we start to make greater use of the expressivity of OWL.

Many of the statements that we have made about pizza are needed to make this inference. For example, if we had not added `:disjoint:` to the subclasses of `PizzaTopping`, we could not make this inference; even though we would know that, for example, a `MozzarellaTopping` was a `CheeseTopping`; by default, the reasoner would not assume that `CheeseTopping` was not a `MeatTopping`, since these two could overlap. There are also some statements in the ontology that we do not use to make this inference. For example, the reasoner does not need to know that a `MargheritaPizza` actually has a `MozzarellaTopping` (the statement (`some` `hasTopping` `MozzarellaTopping`), just that if the pizza has toppings at all, they are only mozzarella or tomato. The semantics of OWL can be subtle, but allow us to draw extremely powerful conclusions.

5.10 Recap

In this chapter, we have described:

- The basic syntax of Tawny-OWL
- New ontologies are created with `defontology`
- Ontologies consist of classes and properties
- Classes describe a set of individuals
- Properties describe relationships between individuals

- Defined classes allow us to make inferences using computational reasoning.

In addition, we have introduced the following semantic statements:

- Subclass relationships
- Disjoint classes
- Covering axioms
- Inverse properties
- Domain and range constraints
- Functional characteristics
- **some** and **only** restrictions, and the **some-only** pattern
- **or** and **not** restrictions

Chapter 6

Highly Patterned Ontologies

Many ontologies contain patterns—that is collections of classes and properties which occur repetitive through the ontology. Dealing with this in many ontology development environments is painful. Tawny-OWL is a fully programmatic environment, however. Patterns are dealt with by writing functions and passing parameters; in otherwords, the same way that we deal with code duplication more generally.

In this Chapter, we will first explore how to use patterns than Tawny-OWL provides explicit support for; then we will move on to show how to modify and extend these patterns in an ontology specific way. Finally, we will show how to use the fully programmatic capabilities of Tawny-OWL to generate a large number of classes in a way that is unique to one ontology.

6.1 Dealing with Patterns

Some ontologies have very few patterns; all the classes and objects are unique. These ontologies tend to be very small, however. Most ontologies describe many similar things with just a few details differing between them. In this chapter, we use the amino-acid ontology – this describes the chemical constituents that make up proteins. There are twenty of these and they are all very similar, with the same properties.

Graphical tools can provide a partial solution to this problem, by supporting the building of these patterns. For instance, Protege had “wizards” to build various patterns. In fact, the first version of the amino-acid ontology was built to demonstrate one of these patterns [?]. This requires extension of the editor for every new pattern, which is acceptable for some generic patterns which can be widely reused, but works badly for patterns

with a narrow scope.

An alternative is to use a language like OPPL [?], which can directly specify patterns and transformations to ontologies. However, this requires the use of two syntaxes or environments – one for “normal” ontological code, and one for patternised. It also presents a maintenance problem – the normal and patternised code is intertwined, so updating a pattern is difficult.

Tawny-OWL take an alternative approach. Instead of providing an alternative language like OPPL, all ontological statements are written in Clojure, which is, itself, an full programming languages. Patterns can be built straight-forwardly by writing or using functions; this can be done in a general library for generic patterns, shared between ontologies. Or, alternatively, it can be done specifically for individual ontologies, in the same syntax, files and development environment as the normal parts. Updates cease to be a problem; in the worst case scenario, this requires restarting the clojure process. Normally, it does not require even that. In short, with Tawny-OWL patterns become an integral part of ontology development, rather than an external imposition.

In this chapter, we first describe how to use an pre-existing pattern provided by Tawny-OWL, then how to modify this slightly for the amino-acid ontology. Finally, we show how to create a *de novo* patternised section creating several hundred defined classes.

6.2 Creating the Amino Acid Ontology

First, we start with a namespace declaration. This is slightly different from ones used before, as it also **requires** two new namespaces. `tawny.pattern` provides pattern support and one key pattern which forms the core of the amino-acid ontology; `clojure.string` provides string manipulation capabilities which we will use. We also define the new ontology.

```
(ns take.wing.amino-acid
  (:import [org.semanticweb.owlapi.search EntitySearcher])
  (:require
    [clojure.string]
    [tawny.owl :refer :all]
    [tawny.pattern :as p]
    [tawny.reasoner :as r]
    [tawny.util :as u]))

(defontology aao
```

```
:iri "http://www.purl.org/ontolink/aao")
```

First, to explain the domain. Proteins are polymers made up from amino-acid monomers. They consist of a central carbon atom, attached to a carboxyl group (the “acid” amino) and amine group (the “amino” group) a hydrogen and an R group. The R group defines the different amino acids. The different R groups have different physical or chemical properties, such as their degree of hydrophobicity. We call these different characteristics *RefiningFeatures*.

```
(defclass AminoAcid)
```

```
(defclass RefiningFeature)
```

```
(defclass PhysicoChemicalProperty :super RefiningFeature)
```

There are a number of different ways of measuring hydrophobicity; in reality, it is a continuous property rather than a discrete one, but these are hard to model ontologically. One simple solution to this problem is the *value partition* – we just pick a set of discrete values into which we partition the range. It is the same trick that is used to describe the colours of the rainbow; we force a continuous range into seven colours. Hydrophobicity splits into just two – hydrophobic and hydrophilic.

The full representation of this knowledge as a value partition is fairly complex. First, we define a root class and an object property, with an appropriate domain and range, and declared functional, as one object can be hydrophilic or hydrophobic but not both.

```
(defclass Hydrophobicity :super PhysicoChemicalProperty)
```

```
(defproperty hasHydrophobicity :domain AminoAcid
  :range Hydrophobicity :characteristic :functional)
```

Next we need to define the partition values. We make Hydrophilic disjoint from Hydrophobic. We do not make Hydrophobic disjoint from Hydrophilic because of Tawny-OWLS “define before use” semantics.

```
(defclass Hydrophobic :super Hydrophobicity)
```

```
(defclass Hydrophilic :super Hydrophobicity :disjoint Hydrophobic)
```

Finally, we refine the first partition Hydrophobic to also be disjoint with Hydrophilic and then add a covering axioms to Hydrophobicity.

```
(refine Hydrophobic
  :disjoint Hydrophilic)
```

```
(refine Hydrophobicity
  :equivalent (object-or Hydrophilic Hydrophobic))
```

Of course, as we have already seen, the use of disjoints and covering axioms is so common that Tawny-OWL provides specific support for adding these, in a way which also allows us to avoid the necessity for refining classes after creation. This produces a much neater definition and is a simple example of the use of patterns.

```
(as-subclasses
  (defclass Hydrophobicity :super PhysicoChemicalProperty)
  :disjoint :cover
  (defclass Hydrophobic)
  (defclass Hydrophilic))

(defproperty hasHydrophobicity :domain AminoAcid
  :range Hydrophobicity :characteristic :functional))
```

This is, however, all still fairly long-winded and relatively easy to get wrong. Tawny-OWL, however, allows us to go further with the use of the `defpartition` macro, which allows specification of all the appropriate values at once. It will produce the same axioms as the statements above.

```
(p/defpartition Hydrophobicity
  [Hydrophobic Hydrophilic]
  :comment "The tendency to associate with water."
  :super PhysicoChemicalProperty
  :domain AminoAcid)
```

`defpartition` is a generic pattern and is not specific at all to the amino-acid ontology. It will serve well, but for the amino-acid ontology we need to define a series of further value partitions. They all have the same super class and domain. It would be nice to create a *localised* pattern which hard-codes these values. As `defpartition` is a macro this is slightly more complex than a normal function, but not heavily so. This macro is unlikely to be of use in another ontology because of these hard-coded values, but it is valuable because it saves typing here and safe-guards us against future changes. Being in the same environment, it is easy to do, so we might as well!

```
(defmacro defaapartition [& body]
  '(p/defpartition
    ~@body :super PhysicoChemicalProperty
    :domain AminoAcid))
```

The next value partition is as a result somewhat smaller, as it no longer needs to describe the super class and domain. The size value partition is self-explanatory enough; this could be described in relation to a continuous

physical measurement (such as size in Daltons), but this is not necessary here.

```
(defaapartition Size
  [Small Tiny Large]
  :comment "The physical size of the amino acid.")
```

Finally, we create three more value partitions describing Charge, SideChainStructure and Polarity.

```
(defaapartition Charge
  [Negative Neutral Positive]
  :comment "The charge of an amino acid.")
```

```
(defaapartition SideChainStructure
  [Aliphatic Aromatic]
  :comment "Does the side chain contain rings or not?")
```

```
(defaapartition Polarity
  [Polar NonPolar]
  :comment "The polarity across the amino acid.")
```

Next, we define a set of annotation properties. In the previous Chapter 5, we made some use of a few annotation properties: the label and the comment. But, in OWL, annotation properties are generic. It is possible to define new annotation properties. This is useful here because amino-acids have a long name, such as *Alanine*, and two shorter names – a three letter abbreviation such as *Ala* and finally one letter abbreviation which is shorter, but harder to remember, in this case *A*. These abbreviations are standardized and widely used, so worth describing here.

```
;; annotation properties
(defaproperty hasLongName)
(defaproperty hasShortName)
(defaproperty hasSingleLetterName)
```

Now, we move onto the heart of this amino-acid ontology which is the function which defines a single amino-acid. This is a fairly large definition, but it is fairly repetitive in itself. First we start with the function definition, combined with a few small pre-conditions; these are probably unnecessary in this case, for reasons we will see soon.

```
(defn amino-acid
  "Define a new amino acid. Names is a vector with the long, three letter and
  single amino acid version. Properties are the five value partitions for each
  aa, as a list."
  [names properties]
```

```
{:pre [(= 3 (count names))
        (= 5 (count properties))]}
```

The main part of the amino acid pattern is defined in the next section. The pattern is not that complex – we simply give an amino-acid five properties and three names. However, to achieve this, we use a new feature of Tawny-OWL: the `gem` and the `facet`.

The `defpartition` macro that we saw earlier creates a large number of different classes and a property associated with them. In addition to these logical statements it also defines a *facet* which comprises the *facet values* (i.e. the classes) and the *facet property*; this knowledge is stored in the ontology as annotations and states that the facet values should normally be associated with this property.

This allows us to use the `facet` function which returns much the same as `owl-some`.

```
(=
  (owl-some hasSideChainStructure Aliphatic)
  (facet Aliphatic))
```

This is a minor convenience, of course, when lots of facet values are being used at once is a big advantage. As with `owl-some`, the `facet` function broadcasts – we can call it with as many arguments as we choose.

```
(=
  (list
    (owl-some hasCharge Neutral)
    (owl-some hasHydrophobicity Hydrophobic)
    (owl-some hasPolarity NonPolar)
    (owl-some hasSideChainStructure Aliphatic)
    (owl-some hasSize Small))
  (facet Neutral Hydrophobic NonPolar Aliphatic Small))
```

Not only has the hassle of typing been reduced but so has the risk of error. It is no longer possible to use the wrong property with the wrong class.

The `gem` functions build on top of this idea; these are similar the `class` or `defclass` functions described earlier, but add a new frame, that of the facet. For example, we could define the amino-acid `Valine` as follows:

```
(defgem Valine
  :facet Neutral Hydrophobic NonPolar Aliphatic Small)
```

In the case of the `amino-acid` function, instead we use the `gem` function and capture its return value as part of a `let` block. This is not strictly

necessary as the return value is used only once, but in this case, I think, it increases readability.

```
(let [aa (p/gem (first names)
                :super AminoAcid
                :facet properties
                :label (first names)
                :annotation
                (annotation hasLongName (nth names 0))
                (annotation hasShortName (nth names 1))
                (annotation hasSingleLetterName (nth names 2)))]
```

The last part is not part of the pattern itself. Rather it adds support for *interning*; this is the process by which OWL objects are bound to Clojure symbols. The practical upshot of this is that we (or anyone importing the amino acid ontology) will be able to refer to amino acids using names like `Alanine` rather than being required to use strings inside quotes — `"Alanine"`. This adds (considerable) complexity to the Tawny-OWL definition of the amino-acid ontology, but is probably worth it for ease of downstream use.

To achieve this, we need to return instances of the `tawny.pattern.Named` class, combined with the strings we use to refer to them. In this case, a single amino-acid class gets three names – this is rather unusual but makes sense here.

```
;; and return types for intern
(map p/->Named
     names
     (repeat aa))))
```

We could stop here in terms of generating our ontology. However, here we take two more steps, one mostly to make the input more consistent, so that we would see errors easily, and one to make the amino-acid ontology more usable within the Tawny-OWL environment.

Firstly, we define a function which takes a number of different amino-acid definitions and runs the amino-acid function over them. It then flattens the list of lists that is returned.

```
(defn amino-acids
  [& definitions]
  (apply
   concat
   (map
    (fn [[names props]] (amino-acid names props))
    (partition 2 definitions)))))
```

Finally, we define a macro. This does two things for us. Firstly it provides the convenience of using “bear” words: so `Alanine` instead of `"Alanine"` within the macro itself. A small convenience for a single amino-acid, but a bigger one for all twenty. There are a variety of ways of achieving this – we could use the `tawny.util/quote-tree` macro to covert all the symbols to strings. However, here, we take the slightly more complex route and just turn the first part of the definition into strings. The rest can remain symbols as they are pre-defined. And, secondly, we *intern* the `Named` values turned from the `amino-acid` function; that is we create a new variable, identified by relevant symbol, with a value which is an OWL entity. The practical upshot of this is that later, we can refer to `Alanine` (or `Ala` or `A`) rather than having to use quotes. In terms of the amino-acid ontology itself, this is unnecessary, but it is useful for another ontology importing the amino-acid ontology, so it is worth doing here. In addition and probably more importantly than the convenience, this also provides a degree of safety: attempts, for instance, referring to an amino-acid `B` will fail with an error as this amino-acid does not exist.

```
(defmacro defaminoacids
  [& definitions]
  (let [definitions
        (interleave
         (map
          #(mapv name %)
          (take-nth 2 definitions))
         (take-nth 2 (rest definitions)))]
    `(p/intern-owl-entities
      (amino-acids ~@definitions))))
```

Then, we define all the amino-acid. These have been laid out in alphabetical order, and the properties arranged in a table which means that we can visually check that everything is correct and nothing is missing.

```
(defaminoacids
  [Alanine      Ala A] [Neutral  Hydrophobic NonPolar  Aliphatic Tiny]
  [Arginine     Arg R] [Positive Hydrophilic Polar     Aliphatic Large]
  [Asparagine   Asn N] [Neutral  Hydrophilic Polar     Aliphatic Small]
  [Aspartate    Asp D] [Negative Hydrophilic Polar     Aliphatic Small]
  [Cysteine     Cys C] [Neutral  Hydrophobic Polar     Aliphatic Small]
  [Glutamate    Glu E] [Negative Hydrophilic Polar     Aliphatic Small]
  [Glutamine    Gln Q] [Neutral  Hydrophilic Polar     Aliphatic Large]
  [Glycine      Gly G] [Neutral  Hydrophobic NonPolar  Aliphatic Tiny]
  [Histidine    His H] [Positive Hydrophilic Polar     Aromatic
Large]
```

```

    [Isoleucine      Ile I] [Neutral  Hydrophobic NonPolar  Aliphatic Large]
    [Leucine         Leu L] [Neutral  Hydrophobic NonPolar  Aliphatic Large]
    [Lysine          Lys K] [Positive Hydrophilic Polar     Aliphatic Large]
    [Methionine      Met M] [Neutral  Hydrophobic NonPolar  Aliphatic Large]
    [Phenylalanine  Phe F] [Neutral  Hydrophobic NonPolar  Aromatic
Large]
    [Proline         Pro P] [Neutral  Hydrophobic NonPolar  Aliphatic Small]
    [Serine          Ser S] [Neutral  Hydrophilic Polar     Aliphatic Tiny]
    [Threonine       Thr T] [Neutral  Hydrophilic Polar     Aliphatic Tiny]
    [Tryptophan      Trp W] [Neutral  Hydrophobic NonPolar  Aromatic
Large]
    [Tyrosine        Try Y] [Neutral  Hydrophobic Polar     Aromatic
Large]
    [Valine          Val V] [Neutral  Hydrophobic NonPolar  Aliphatic Small]
)

```

Finally, we clean up by ensuring that all amino-acids are disjoint from each other. We could do this earlier in the `amino-acids` function, but as this function only needs to be run once, it makes little difference.

```
(apply as-disjoint (subclasses AminoAcid))
```

6.3 Defining the Amino Acids

We saw earlier, while considering pizza, that it is possible to create defined classes (see Section 5.9). For the amino-acid ontology, this is also tremendously useful because we can effectively use this to query it. Consider, for example, this definition of `LargeAminoAcid`.

```
(defclass LargeAminoAcid
  :equivalent (owl-some hasSize Large))
```

This is fine, of course, but is also very slow, as there are a lot of potential classes that we could create. As well as one for each of the twelve values in our five value partitions, we also need all of the permutations of these, which makes quite a few classes.

Of course, being fully programmatic, calculating permutations in Tawny-OWL is a simple enough task; so, why not build all of these defined classes programmatically?

This is reasonably straight-forward; first, we need a definition for a defined class; this will take a list of partition values. The pattern simply involves making existential (`owl-some`) restrictions to all of the partition values using the appropriate object property; we can achieve this using the

facet function that we saw earlier. We form the name of the class from the names of the partition values.

```
(defn amino-acid-def [partition-values]
  (let [name
        (str
         (clojure.string/join
          (map
           #(.getFragment
            (.getIRI %))
           partition-values))
         "AminoAcid")]
    exist (p/facet partition-values)])
```

Then finally we create the class and package it with its name. As with our previous amino-acid definition, this function has a return value which would allow it to be used to intern the classes created, although we do not actually use that facility here.

```
(p/->Named
 name
 (owl-class
  name
  :label name
  :equivalent
  (owl-and AminoAcid exist))))
```

Calculating a cartesian product is relatively easy in Clojure using the swiss-army knife `for` list comprehension.

```
(defn cart [colls]
  (if (empty? colls)
    '())
    (for [x (first colls)
          more (cart (rest colls))]
      (cons x more))))
```

We combine all of these together to create all of the defined classes.

```
;; build the classes
(doall
 (map
  amino-acid-def
  ;; kill the empty list
  (rest
   (map
    #(filter identity %)
    ;; combination of all of them
```

```
(cart
  ;; list of values for each partitions plus nil
  (map
    #(cons nil (seq (direct-subclasses %)))
    ;; all our partitions
    (seq (direct-subclasses PhysicoChemicalProperty))))))
```

Finally, we check to see whether everything has worked. For this, we will need to use a reasoner, so first we choose a reasoner and check the consistency of our ontology.

```
(r/reasoner-factory :hermit)
(r/consistent?)
```

We can also investigate the classes that we have created. None of the created classes should have any asserted subclasses, which we can check, by looking at one.

```
(subclasses
  (owl-class "SmallAminoAcid"))
```

However, we see a totally different picture with the reasoner. We can first check for inferred subclasses.

```
(r/isubclasses
  (owl-class "SmallAminoAcid"))
```

We might have expected to just see a few as there are only 20 amino-acids, but actually, there are 113 of them. The reason for this is that the reasoner determines the subclass relationships between the defined classes as well as with the named amino-acids: so, for instance, an `HydrophobicSmallAminoAcid` is necessarily also a `SmallAminoAcid` so appears as a subclass. This demonstrates the power of using a computational reasoner; while the conclusions that it reaches are not, in this case, difficult to calculate by hand, with so many classes they would be laborious.

Unfortunately, in this case, they also hide the answer that we are really interested in. In a less programmatic tool, we would be stuck, but this is not a problem in Tawny-OWL; we just filter the defined classes from the result as follows.

```
(filter
  #(not (EntitySearcher/isDefined % aao))
  (r/isubclasses
    (owl-class "SmallAminoAcid")))
;; => ([Class 0x6f148b89 "Valine"@en] [Class 0x4c949f3e "Proline"@en]
;;      [Class 0x57f95b76 "Glutamate"@en] [Class 0x784dcd0 "Asparagine"@en]
;;      [Class 0x4c07576a "Aspartate"@en] [Class 0x24024cbb "Cysteine"@en])
```

And the end result? There are six small amino-acids!

With Tawny-OWL it is straight-forward to implement new patterns building a very large number of classes at once; the amino acid ontology is a nice example of this. At the current time, we do not really know how common the requirement is for this sort of ontology; most ontologies in existence are not heavily patternized. But, then, perhaps this is part because the tools for generating patterns were not integrated into our ontology development process; patternized ontologies are not common because they are just too painful to produce.

Even aside from heavily patternized ontologies, this chapter also shows that Tawny-OWL can be easily extended even within the scope of a single ontology. The `defaapartition` macro is only useful here. But, it is easy to write, reduces duplication and increases consistency of the end ontology. Most ontologies have this form of repetition. With Tawny-OWL, managing this repetition becomes the task of the computer and not the task of the human, which is as it should be.

6.4 Recap

In this chapter, we have described:

- The `tawny.pattern` namespace.
- The Value-Partition design pattern
- Gems and Facets
- A macro expanding the value-partition.
- An amino-acid function
- Intern with `intern-owl-entities`
- A highly patternized part of the ontology.