## Datasets

Social scientists often work with datasets that are structured as a collection of records, where each record consists of multiple fields, and each field has an identifier and a value. Such data is in a tabular format (or more simply, it is a table). Abstractly, this structure is naturally modeled as a list of associations, where each association represents a single record, and where the keys of the association are the field identifiers. For example, the following three associations could represent three records in a data set.

In[ $]:=$ assoc01 = <|"first" $\rightarrow$ "John", "last" $\rightarrow$ "Doe", "h1" $\rightarrow$ 50, "h2" $\rightarrow$ 30|>;
assoc02 = <|"first" $\rightarrow$ "Jane", "last" $\rightarrow$ "Doe", "h1" $\rightarrow$ 30, "h2" $\rightarrow 50 \mid>$;
assoc03 = <|"first" $\rightarrow$ "Signor", "last" $\rightarrow$ "Rossi", "h1" $\rightarrow 46$, "h2" $\rightarrow 45 \mid>$;
This section briefly considers a WL data type that can be very similar to a list of associations: the Dataset. It provides the same natural representation of tabular datasets, with additional advantages for transformation, selection, and aggregation. (For more details see the Wolfram Language Guide entitled Computation with Structured Datasets.)

## Creating Datasets

The Dataset command converts a list of associations into a unified structure that is easily queried and manipulated. In a Mathematica notebook such a dataset has a convenient visual display.

| Out $[0]=$ | $\begin{gathered} \frac{\text { Expression }}{\text { ds01=Dataset [\{ }} \\ \text { assoc01, } \\ \text { assoc02, } \\ \text { assoc03 } \end{gathered}$ | Result |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | first | last | h1 | h2 |
|  |  | John | Doe | 50 | 30 |
|  |  | Jane | Doe | 30 | 50 |
|  |  | Signor | Rossi | 46 | 45 |

Such a dataset is essentially a convenient wrapper around the list of associations. In fact, whenever needed, the Normal command can retrieve the list of associations from such a dataset. Furthermore, many of the manipulations supported by such datasets are readily achievable with a list of associations. However, datasets support particularly convenient syntax for common manipulations.

Most often, dataset creation involves import from an external file. The SemanticImport command excels at creating data sets from external data files, such as spreadsheet files. (The WL documentation provides extensive details.) In order to produce a self-contained example, the following illustration uses the closely related SemanticImportString command, which operates directly on strings. Even without additional clues, Mathematica recognizes that the string data is in CSV format.

| Expression |  |  |  | Result |
| :--- | :--- | :--- | :--- | :--- |
| SemanticImportString [ <br> "first, last, h1, h2 | first | last | h1 | h2 |
| John, Doe, 50, 30 <br> Jane, Doe, 30,50 <br> Signor, Rossi, 46,45"] | John | Doe | 50 | 30 |
|  | Jane | Doe | 30 | 50 |
|  | Signor | Rossi | 46 | 45 |

## Filtering and Recoding Datasets

From a given dataset, researchers often work with a smaller dataset comprising only those records that satisfy some criterion. Recall that this process is called selective set building, filtering, or subsetting. Criterion-based filtering of datasets is a very common need. The Select command can perform dataset filtering: apply it to a dataset and an appropriate predicate (i.e., a function that returns True iff a record satisfies our criterion).

For example, suppose that from ds01 we wish to keep only those records where the $\mathbf{h 1}$ and $\mathbf{h 2}$ fields sum to less than 90 . Begin this task by implementing an appropriate selector, as follows.

```
In[0]:= select01 = Select[#h1 + #h2 < 90 & ];
```

To understand this selector, recall that when associations that have strings as keys, functions operating on them can refer by key name to the values. The example also illustrates the operator form of Select, which can be particularly convenient when the same criterion will be used to subset several datasets. (See the documentation for details.) This selector would work just well on a list of associations. However, when applied to a dataset the result is a dataset, which in a notebook has a nice display. Interestingly, in addition to the more obvious syntax in the following example, WL allows ds01[select01] as an alternative query syntax.

| Expression | Result |  |  |  |
| :--- | :--- | :--- | :--- | :--- |
| select01[ds01] | first | last | h1 | h2 |
|  | John | Doe | 50 | 30 |
|  | Jane | Doe | 30 | 50 |

Substitutive set building is sometimes called transformation or recoding. For datasets, the Map command largely covers substitutive set building. One may map over the records of a dataset to produce a new dataset. Typically, dataset transformations retain some kind of unique record identifier, precluding the creation of exact duplicates. In a WL dataset, the records are ordered, and that order is retained after mapping.

Remember that functions that transform associations have direct access to the association keys. For example, the following expression defines a function sub01 that accesses four fields of an association and then creates a new association.
$\ln [-0]=$

```
sub01 = <| "first" -> #first, "last" -> #last, "total" -> #h1 + #h2|> &;
```

This facility implies that Map can create recoded datasets with easily understood transformations. For example, recalling the slash-atmark (/@) shorthand for Map, the following example produces a new dataset that holds only names and totals for each record of the original dataset. To understand this, recall that this dataset is essentially a list of associations, so that this code maps the substitution function across that list and produces a new list of associations. In fact, one may proceed in exactly this way, sacrificing only the convenient display of the result. Interestingly, in addition to the more obvious syntax in the following example, WL allows ds01 [All, sub01] as an alternative query syntax.

| Expression | Result |  |  |
| :--- | :--- | :--- | :--- |
| sub01 /@ ds01 | first | last | total |
|  | John | Doe | 80 |
|  | Jane | Doe | 80 |
|  | Signor | Rossi | 91 |

## Queries for Recoding and Selection

In database terminology, selective or substitutive set building performs a query, which retrieves information from a dataset. WL correspondingly provides the Query command for producing query operators. Applying a query operator to a dataset produces a subset or a transformation (or a transformed subset). The query syntax is extremely flexible, and queries may be complex. This subsection illustrates a few simple queries.

As initial example of queries, consider the filtering and recoding examples from the previous subsection. The query to implement the filtering example is Query [select01]. The query to implement the recoding example is Query [All, sub01]. Each of this produce a function that may be applied to a data set (or a list of associations) to produce the associated filtering or recoding. In addition, they can be readily combined, as follows. After selecting only the records of interest (rather than all of them), each record is transformed.

Out $[0]=$

| Expression | Result |  |  |
| :--- | :--- | :--- | :--- |
| Query[select01, sub01] @ ds01 | first | last | total |
|  | John | Doe | 80 |
|  | Jane | Doe | 80 |

As a convenient shorthand for such a query, a data set can be applied directly to the query components.

Out [0]=

| Result |  |  |  |
| :--- | :--- | :--- | :--- |
| dspression $[$ select01, sub01] | first | last | total |
|  | John | Doe | 80 |
|  | Jane | Doe | 80 |

As another example of recoding a dataset, consider the selection of a subset of the fields from every record. First characterize set of records to process (here, all of them), and then list the desired columns (by name). Here instead of applying Query [All, \{"h1", "h2"\}] to the dataset, use the specialized query syntax from the previous example. (An alternative query to achieve this result is KeyDrop[\{"first","last"\}].)

| Expression |  | Result |
| :--- | :--- | :--- |
| hvals $=$ <br> ds01 [All, \{"h1", "h2" \}] | h1 | h2 |
| 50 | 30 |  |
| 30 | 50 |  |
|  | 46 | 45 |

Recall again that functions applied to associations can make direct use of the association keys, which facilitates easy creation of transformed datasets with Map. For example, the following function will append to an associations a new key ("total") with a value that is the sum of the values associated to the "h1" and "h2" keys.

```
sub02 = Append[#, "total" -> #h1 + #h2] &;
```

It is quite possible to map this function across the data01 dataset. In this fashion, substitutive set building can add fields. When recoding datasets, a more idiomatic alternative is to create an equivalent query: once again use Query with the transformation as the second argument. The following example again does this by means of the specialized query syntax; it use sub02 to append a "total" column to the dataset.

| Result |  |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :---: |
| dspression $=$ ds01[All, sub02] | first | last | h1 | h2 | total |  |
|  | John | Doe | 50 | 30 | 80 |  |
|  | Jane | Doe | 30 | 50 | 80 |  |
|  | Signor | Rossi | 46 | 45 | 91 |  |

As noted before, the Query command is remarkably flexible. For example, as explored in the next subsection, queries can sort the data set on arbitrary criteria. An interesting and surprising application of dataset queries is that LinearModelFit can be used as a query operator, after removing the field
names. To discard the dataset headers, apply the Values command. This produces a headerless rectangular dataset, which essentially wraps a rectangular list of lists rather than a list of associations. (Use the Normal command to produce the underlying list of lists.)

Out[ $[=$

| Expression | Result |
| :--- | :--- |
| hvals [LinearModelFit $[\#, ~ x, ~ x] \&]$ | FittedModel $[75.4167-0.803571 \mathrm{x}$ |

Later discussions treat linear regression in more detail. The Wolfram Language How To entitled Perform a Linear Regression provides a useful introduction.

## Partitioning and Classification

A partition of a set $X$ is a collection of non-empty, pairwise-disjoint subsets whose union is $X$. Each of these subsets is called a block. Recall that a collection of sets is pairwise-disjoint if the intersection of any pair of the sets is empty, so different blocks of a partition have no elements in common. The simplest interesting partition is a two-block partition. Two-block partitions are naturally formed by dividing set elements into those that satisfy a certain property and those that do not. Whenever selective set building picks a subset of items that satisfy some predicate, one may produce a corresponding partition by additionally creating the complement of that subset.

Since a list without duplicates may nicely represent a finite set, partitioning such a list can illustrate partitioning a set. The following example uses TakeDrop and Partition to produce some arbitrary blocks from a small list of numbers. The basic form of the TakeDrop command takes as arguments a list and an initial sequence length. It partitions the list into two sublists: an initial sequence, and the remainder of the list. The second argument can alternatively be a list of two integers, which specify the start index and stop index of a sublist to take. The Partition command offers a different approach to partitioning: it can partition a list into sequential sublists of a common length. The following example uses the two-argument form of Partition, where the first argument is a list and the second argument is the length of the sublists. In order to avoid discarding terminal elements when the list is not evenly divisible, use the UpTo command in the second argument.

Out $[0]=$

| Expression | Result |
| :--- | :--- |
| n7=Range $[7]$ | $\{1,2,3,4,5,6,7\}$ |
| TakeDrop $[\mathrm{n} 7,3]$ | $\{\{1,2,3\},\{4,5,6,7\}\}$ |
| TakeDrop $[\mathrm{n} 7,\{3,5\}]$ | $\{\{3,4,5\},\{1,2,6,7\}\}$ |
| Partition $[\mathrm{n} 7$, UpTo [3] ] | $\{\{1,2,3\},\{4,5,6\},\{7\}\}$ |

This example shows that, given a list that represents a finite set, TakeDrop or Partition can produce a list of lists that represents a particular set partition. However, social scientists more commonly need a partition that is based on properties of the elements. Such a partition is called a categorization or a classification of the elements, where the classification typically derives from a classifier function.

## Use of GroupBy

The simplest two-argument form of the GroupBy command accepts as arguments a list to be classified and a classifier function. The result is an association from categories in the range of the classifier
function to the lists of elements in each category, representing a one-way classification of the data. For example, a set of households might be classified by household size. The following functions serve as classifier examples. The first maps each integer to a single classification, either "even" or "odd". The second maps each integer to a single classification, either "div3" or " $\neg$ div3"; this classifies any integer as divisible by 3 or not. The third maps each integer to a single classification, either "div4" or "っdiv4"; this classifies any integer as divisible by 4 or not. Clearly, some of these classifications can overlap, as discussed below.

```
div2 = item \mapsto If[EvenQ[item], "even", "odd"];
```

div3 = item $\mapsto ~ I f[0==$ Mod[item, 3], "div3", " $\operatorname{div3"];~}$
div4 = item $\mapsto ~ I f[0==$ Mod[item, 4], "div4", " $\operatorname{div4"];~}$

When applied to a set of elements, categorization with GroupBy represents the inverse relation of the classifier function on a set. For example, apply the div2 classifier to the first seven positive integers, as follows.

| Expression | Result |
| :--- | :--- |
| gb2 $=$ GroupBy $[\mathrm{n} 7$, div2 $]$ | $\langle \|$ odd $\rightarrow\{1,3,5,7\}$, even $\rightarrow\{2,4,6\}\rangle$ |

In a Mathematica notebook, applying the Dataset command to the resulting association produces a convenient tabular display.

Out[ $\circ$ ]=

| Expression |  | Result |
| :--- | :--- | :--- |
| ds2 $=$ Dataset $[$ gb2 $]$ | odd | $\{1,3,5,7\}$ |
|  | even | $\{2,4,6\}$ |

As a second simple example, use the one argument form of GroupBy, which produces a grouping operator. (Recall that the at-sign operator is the prefix notation for function application.)

| Result |  |  |
| :--- | :--- | :--- |
| Dataset @ GroupBy[div3] @ n7 | $\neg \operatorname{div} 3$ | $\{1,2,4,5,7\}$ |
|  | div3 | $\{3,6\}$ |

A single classification can partition a dataset. A second classification can then refine this partition. That is, partition blocks can themselves be partitioned, resulting in a refined partition of the original set. (Partition $\Pi^{\prime}$ is a refinement of partition $\Pi$ iff every block of $\Pi$ ' is included in a block of $\Pi$.)

It is possible to sequentially refine a partition by mapping a second GroupBy operator across the values of an initial grouping. However, the GroupBy command simplifies this: it accepts a list of classifiers that are sequentially applied. The following example illustrates this nested categorization by producing a two-way classification. The result is a multilevel association: an association whose values are in turn associations. Once again, the Dataset command can produce a convenient tabular display of the result. The outer association keys are used as row headers. When the inner associations share keys, as they do here, the Dataset command typically displays these keys as column headers.
(Refined control of the display of datasets is beyond the scope of this book, but see below for a few hints.)

## Block Size as a Dataset Query

Social scientists often care about the sizes of the partition blocks, since these are the frequency counts produced by the categorization. A one-way frequency table displays categorical data as a list of categories and their frequency of occurrence in a dataset. Mapping Length across a one-way categorization produced by GroupBy will produce the information for a one-way frequency table (as an association from categories to counts). However, when working with data set objects, it is more natural to produce the length of each block by means of a query. Construct the query with the following reasoning: for each category in a one-way categorization, we want the total number of items in that category. This suggests the query Query [All, Length]. Try this out on the previous even-odd classification dataset. In a Mathematica notebook, the result displays as a simple one-way table.

| Respression |  |  |
| :--- | :--- | :--- |
| ds2[All, Length] | odd | 4 |
|  | even | 3 |
|  |  |  |

The same approach can create a two-way frequency table, which shows frequency counts for each possible pair of classifications. Recall that a two-way categorization using GroupBy creates a multilevel association, which is an association whose values are also associations. A frequency table reports the number of items for each value of the inner association. This suggests the query

Query [All, All, Length]. Try this out on the previous two-way classification dataset. In a Mathemat ica notebook, the result displays the element count for each block of the resulting partition of the dataset. It is a frequency table for data described by two categorical variables, which is often called a two-way table, a two-dimensional cross-tabulation, or a contingency table.

| Expression |  |  | Result |
| :--- | :--- | :--- | :--- |
| ds23[All, All, Length] |  | $\neg \operatorname{div3}$ | div3 |
|  | odd | 3 | 1 |
|  | even | 2 | 1 |

## Underneath Query

Query provides a convenient interface for dataset manipulations, but it can be helpful to recall that underneath it is just applying functions at various levels of the dataset. The easiest way to see this is to reveal the underlying operations with the Normal command. (The results involve the operator forms of GroupBy and Map.)

Out[ $\cdot 0$ ] $=$

| Expression | Result |
| :--- | :--- |
| Normal @ Query[GroupBy[f]] | GroupBy[f] |
| Normal @ Query[All,f] | Map[f] |
| Normal @ Query[All,All,f] | Map[Map[f]] |

This means that Map command can also produce the previous result, which again displays the power of Map. Nevertheless, the use of queries is idiomatic when working with datasets.

The remaining subtlety is that Query classifies dataset operations as descending or ascending. Given a sequence of operations in a query, the descending operation are applied in order (at deeper and deeper levels) and then the ascending operations are applied in reverse order at higher and higher levels. Crucially, user-defined functions are ascending. See the documentation of Query for details.

## Display Issues

The example above produces a nice cross-tabulation display with little effort. In the presence of empty categories, a nice display involves a bit more work. For example, pick a different secondary classifier: divisibility by 4 instead of divisibility by 3 . The result is still a partition of the set, but now nothing is listed for the empty category (odd and divisible by 4). Using the Dataset command to produce a convenient categorical display is still acceptable, but the hierarchical display is not as easy to decipher as a two-way table.


In this case, it is possible to produce a display comparable to the previous two-way table by providing a default value for every inner group and then updating it based on the data. For example, map an association providing default values across every row of the dataset. (The default values must come first.) Note that the result is no longer a true partition, because this adds an empty list.

| Expression | Result |  |  |
| :---: | :---: | :---: | :---: |
| ```provideDefaults = < "div4"->{},"\negdiv4" }->{},#\|>& ds24[All,provideDefaults]``` |  | div4 | $\neg$ div4 |
|  | odd | \{\} | $\{1,3,5,7\}$ |
|  | even | \{4\} | $\{2,6\}$ |

To understand how this works, peer inside the dataset wrapper with the Normal command. This dataset is essentially an association whose values are also associations. Recall that applying Map to an association transforms the values, not the keys. For example, the key "odd" associates to the value $\langle | " \neg$ div4" $\rightarrow\{1,3,5,7\} \mid>$. Applying provideDefaults to this value produces $\langle |$ "div4" $\rightarrow\}, " \neg \operatorname{div4"\rightarrow \{ 1,3,5,7\} |\rangle \text {.Withthisunderstanding,itisclearthatmapping}}$ provideDefaults over the dataset $\mathbf{d s} 24$ will provide these defaults wherever needed. The example does this, using the specialized query syntax for datasets.

As of Mathematica version 13 , control of dataset display remains tricky. It is affected by inferred type information, which is beyond the scope of this book. Sometimes the above trick fails to produce a twoway display rather than a hierarchical display. Applying Transpose twice to the dataset sometimes forces the two-way display. An alternative is to use a dataset for recoding, filtering, and aggregation, and then subsequently extract the results for use with TableForm or Grid.

```
dta = Normal@ds24[All, Map[Length] @* provideDefaults];
(* get the nested associations (with defaults) *)
rowHeaders = Keys@dta; colStubs = Keys@First@Values@dta;
(* extract the stubs & headers *)
values = Outer[dta, rowHeaders, colStubs]; (* extract the data *)
```

| Expression | Result |  |  |
| :--- | :--- | :--- | :--- |
| TableForm[values, |  | div4 | ᄀdiv4 |
| TableHeadings $\rightarrow$ \{rowHeaders, colStubs\}] | odd | 0 | 4 |
|  | even | 1 | 2 |

