Extending iSEE

Kevin Rue-Albrecht, Federico Marini, Charlotte Soneson, and Aaron Lun2019-12-10

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Preface

The Bioconductor *iSEE* package provides functions for creating an interactive graphical user interface (GUI) using the RStudio *Shiny* package for exploring data stored in *SummarizedExperiment* objects, including row- and column-level metadata (Rue-Albrecht et al., 2018). In this book we describe how to create web-applications that leverage builtin panels and develop new ones.

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Panel classes

1.1 Overview

The types of panels available to compose an iSEE app are defined as a hierarchy of S4 classes.

```
• Panel*

- DotPlot*

* ColumnDotPlot*

· RedDimPlot

· ColDataPlot

· FeatAssayPlot

* RowDotPlot*

· RowDataPlot

· SampAssayPlot

- Table*

* RowTable*

· RowStatTable

* ColumnTable*

· ColStatTable

- HeatMapPlot
```

Some of those classes are "virtual" (indicated by *), meaning that they cannot be directly instanciated as panels in the GUI. Instead, virtual panel classes define families of panels that share groups of properties. Virtual classes are meant to be used as the parent of one or more concrete classes. In contrast, concrete classes must define fully-functional panels that can be embedded in a GUI, interact with other panels, receive and process data, and generate an output such as a plot or a table, accompanied by a code chunk to display in the code tracker for reproducibility.

1.2 The Panel class

The top-most class is called Panel. It is a virtual class that defines the core properties common to any panel - existing or future - that may be displayed in the interface.

PanelId	Integer index indicating the i th panel
	of a given type.
PanelHeight	Height of the panel, in pixels.
PanelWidth	Width of the panel, an integer value
	indicating the number of columns to
	use, from 1 to 12.
SelectBoxOpen	Logical value indicating if the
	Selection parameters box of the
	panel is open when the app starts.
SelectByPlot	Encoded name of the panel from
-	which to receive a selection of data
	points.
SelectMultiType	Keyword indicating the method to
	deal with multiple incoming
	selections of data points.
SelectMultiSaved	Integer index indicating a single
	data point selection to use, among
	multiple incoming selections.

1.3 The DotPlot and Table panel families

The Panel virtual class is directly derived into two major virtual sub-classes:

- DotPlot
- Table

Those classes introduce properties that are specific to distinct subsets of panel types.

The DotPlot class introduce parameters specific to panels where the output is a ggplot object and each row in the data-frame is represented as a point in a plot.

The Table class introduce parameters specific to panels where the main output is a data-frame directly displayed as a table in the GUI.

In addition, the HeatMapPlot class defines a special panel class that directly extends the Panel class, as it introduces a set of parameters distinct from both the DotPlot and Table panel families. This panel type is described in further details in a separate section below.

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- 1.8 Built-in ColumnTable panel classes
- 1.9 Built-in RowTable panel classes
- 1.10 The HeatMapPlot panel class

This type of panel introduces parameters specific to panels where the output is a heat map, with each row representing a feature and each column representing a sample in the se object.

The app server

- 2.1 Reactive objects
- 2.2 Persistent (non-reactive) objects

2.3 The app memory

The app memory is a list of instances created from available panel classes, which defines the order in which individual panels are displayed in the GUI.

2.4 The panel API

2.4.1 .cacheCommonInfo

Each individual panel type (e.g., $Reduced\ dimension\ plot$) and family of panel types (e.g., $Column\ dot\ plot$) defines a <code>.cacheCommonInfo</code> function.

This function is called for each panel instance in memory when the app is initialized. It allows the app to efficienly compute a single time common information that only depends on the input se object, and may be frequently reused during the runtime of the app.

Following the hierarchy of panel types, each call to the signature takes a panel instance x and the se object, and caches common information relevant to all instances of that panel type in the se object itself, before calling callNextMethod() to invoke the next parent signature.

The top-most signature - for the Panel class - returns the se object that contains all the cached information.

Note that this function only populates the cache for the first panel of each type; it is a no-op if the common cache has already been initialized.

2.4.2 .refineParameters

Each individual panel type (e.g., *Reduced dimension plot*) and family of panel types (e.g., *Column dot plot*) defines a .refineParameters function.

This function is called for each panel instance in memory when the app is initialized, and also when a new panel is added to the GUI. It inspects the parameters of a given panel instance, and replaces invalid parameters with sensible values for a given se object.

Following the hierarchy of panel types, each call to the signature takes an instance x and the se object, and first calls callNextMethod() to invoke the next parent signature, to refine generic parameters before processing specific ones.

The called signature ultimately returns the updated instance panel x, or NULL if the panel instance is not available for this app.

2.5 Initialization of the app server

The app server is initialized as soon as a valid **se** object is provided. This can be either in the call to **iSEE(se)** or using the Shiny file upload button in apps that were launched without providing the **se** arguments, e.g., **iSEE()**.

The initialize_server function takes the se object and the list holding reactive values used to trigger re-rendering of the GUI, as described above.

The very first step invokes the function .sanitize_SE_input on the se object. This function coerces the se to SingleCellExperiment, flattens nested DataFrames, adds row and column names, and removes other non-atomic fields. In addition, it also sanitizes the SingleCellExperiment object by moving internal fields into the column- or row-level metadata, making them visible in the Column statistics table and Row statistics table panels, respectively. The function returns both the sanitized se object that will be used by the app, and the list of R commands that will be displayed in the code tracker for users.

Next, the server invokes the checkColormapCompatibility function. This function takes the se object and the optional colormap provided to iSEE(), and carries out a number of compatibility checks between the two objects. The function collects a character vector of issue messages that are displayed - if any - as warning messages in GUI during initialization.

Next, the .cacheCommonInfo and .refineParameters are successively invoked on each panel instance initialized in the app memory. As described in a separate section above, the first function precomputes and caches information specific to the se object and frequently used throughout the runtime of the app. The

second function ensures that each panel instance is initialized with valid parameters; it replaces any invalid parameters with sensible values for a given se object.

Next, persistent (non-reactive) objects are initialized:

- the app memory (see this section)
- the count of panels of each type, used to assign increasing ID to new panel instances
- the list of commands to display in the code tracker for each panel instance
- the list of data point coordinates selectable in each panel instance¹
- a list of miscellaneous cached information²

 $^{^{1}\}mathrm{Data}$ points downsampled for rendering speed performance remain selectable, even though

they are not visible in the plot. 2 The plot that contain the legend keys of Heatmap panels is currently cached as miscellaneous information retrieved separately when rendering the GUI.

The plotting API

3.1 .getPlottingFunction

Each panel type available for use in the GUI defines a .getPlottingFunction.

This function is called within .createRenderedOutput, which is triggered by observers when the value of the panel input widgets are changed by users, or when a new panel is added to the GUI.

The .getPlottingFunction function inspects the parameters for a given panel instance, and uses the app memory of all active panels and parameters, the coordinates of data points in each plot panel, the se object, and the colormap to generate all the information necessary to render the outputs of this panel and those that depend on it.

For DotPlot panels, the output is a list that includes:

- the list of commands to display in the code tracker
- the coordinates of data points in the plot
- the ggplot object

For Table panels, the output is a datatable.

For the HeatMap panel, the function does not return any value. Instead it sets relevant elements in the output object of the Shiny session.

Developing new panels

First things first, we need to load the iSEE package for this chapter.

library(iSEE)

4.1 Create a new S4 class

In the chapter Panel classes, we saw how each type of panel is defined as an S4 class, organised in a hierarchy that allows new panel classes to inherit sets of the properties and functionality from parent classes.

Therefore, developing a new panel starts with the creation of a new class.

The choice of a parent class for the new panel depends on the properties that we want that new panel to have. For instance, let us say that we want to define a new panel that has all the functionality of the *Reduced dimension plot* panel type, but summarizes data into a layer of hexagonal bins instead of showing each individual data point. To do so, we declare our new class with a new unique name, *e.g.* RedDimHexbinPlot, that contains the builtin panel class RedDimPlot.

setClass("RedDimHexbinPlot", contains="RedDimPlot")

Bibliography

Rue-Albrecht, K., Marini, F., Soneson, C., and Lun, A. T. L. (2018). isee: Interactive summarized experiment explorer. F1000Res, 7:741.