

Melbourne Bioinformatics Seminar

Hatching a plot (and more) on the command line: part 3

Bernard Pope
Victorian Health and Medical Research Fellow
Melbourne Bioinformatics
The University of Melbourne, Australia

Another Hatch talk?

- ❖ The ~~beatings~~ talks will continue until ~~morale improves~~ someone else uses hatch

Recap

- Hatch is a **command line** tool for **analysing** and **visualising** data.
- Input is tabular data in CSV or TSV format.
- Output is (one or both of):
 - plot(s)
 - transformed tabular data in CSV or TSV format
- Built on top of pandas, scikit-learn, numpy, matplotlib, seaborn.

Simple example

```
cat iris.csv | hatch pretty
```

sepal_length	sepal_width	petal_length	petal_width	species
5.1	3.5	1.4	0.2	setosa
4.9	3.0	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5.0	3.6	1.4	0.2	setosa
...
6.7	3.0	5.2	2.3	virginica
6.3	2.5	5.0	1.9	virginica
6.5	3.0	5.2	2.0	virginica
6.2	3.4	5.4	2.3	virginica
5.9	3.0	5.1	1.8	virginica

[150 rows x 5 columns]

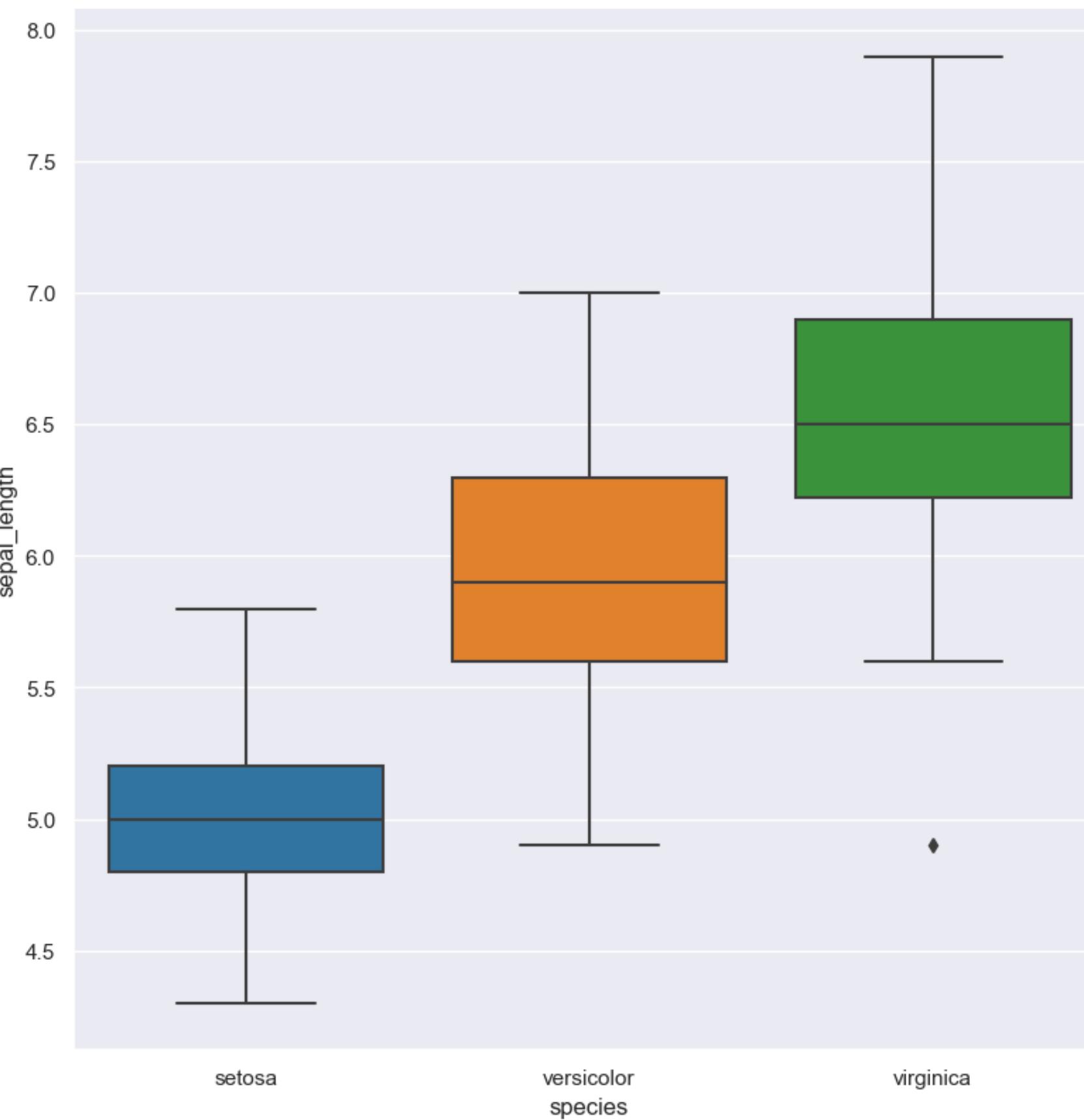
Simple example

```
cat iris.csv | hatch describe
```

	sepal_length	sepal_width	petal_length	petal_width	species
count	150.000000	150.000000	150.000000	150.000000	150
unique	NaN	NaN	NaN	NaN	NaN
top	NaN	NaN	NaN	NaN	NaN
freq	NaN	NaN	NaN	NaN	NaN
mean	5.843333	3.054000	3.758667	1.198667	NaN
std	0.828066	0.433594	1.764420	0.763161	NaN
min	4.300000	2.000000	1.000000	0.100000	NaN
25%	5.100000	2.800000	1.600000	0.300000	NaN
50%	5.800000	3.000000	4.350000	1.300000	NaN
75%	6.400000	3.300000	5.100000	1.800000	NaN
max	7.900000	4.400000	6.900000	2.500000	NaN

Simple example

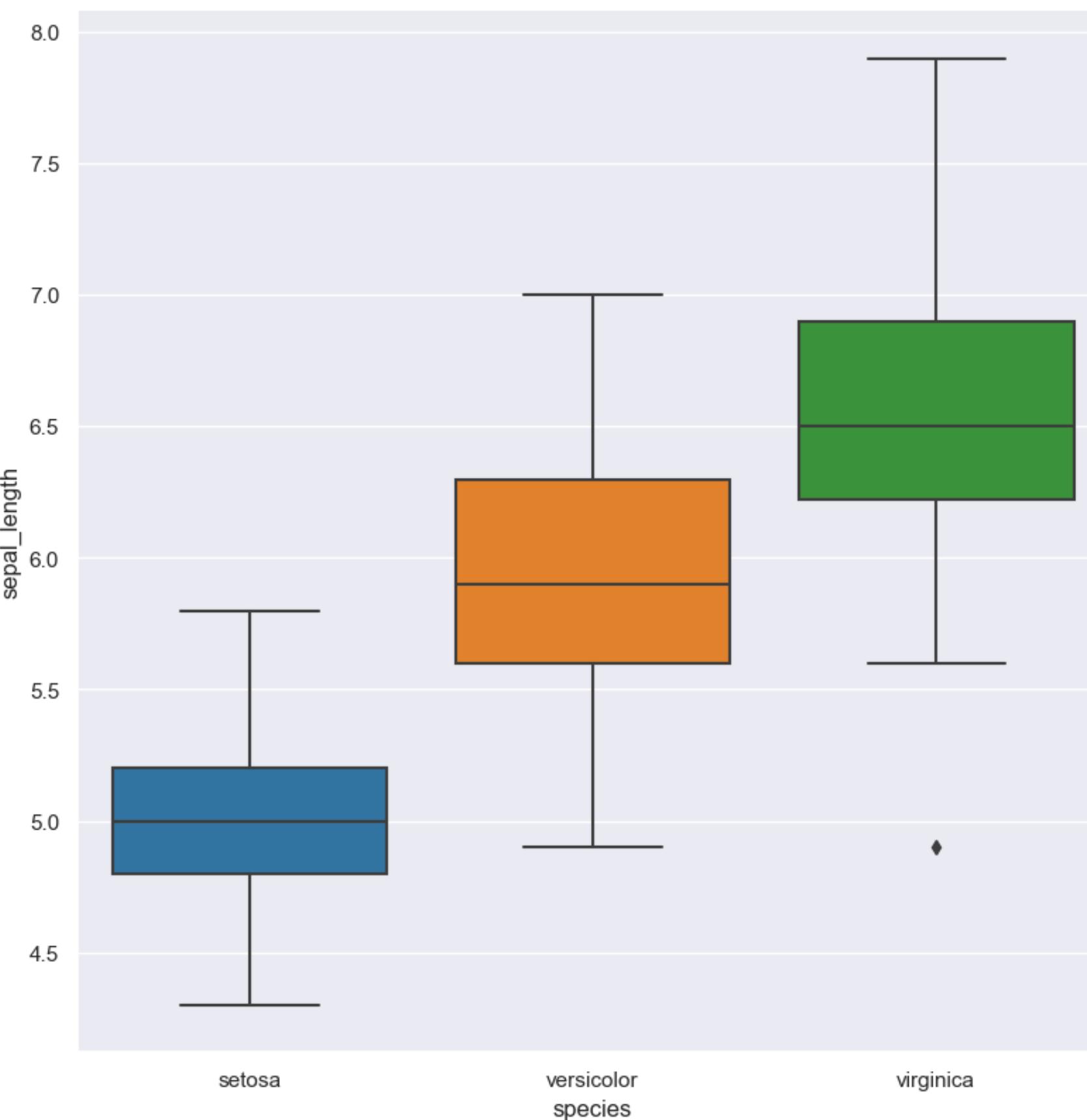
```
cat iris.csv | hatch box -x species -y sepal_length
```



output is written to
hatch.species.sepal_length.box.png

Equivalently

```
hatch box -x species -y sepal_length < iris.csv
```

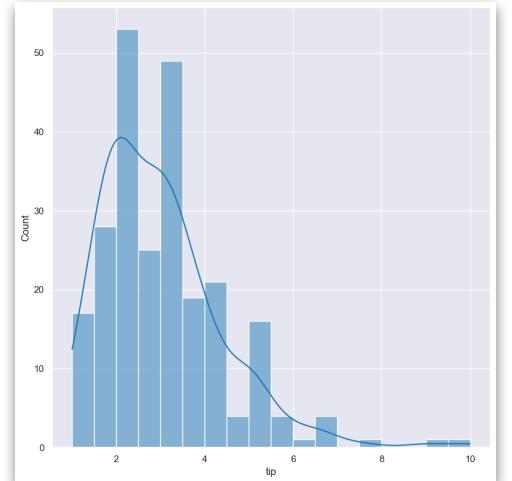


output is written to
hatch.species.sepal_length.box.png

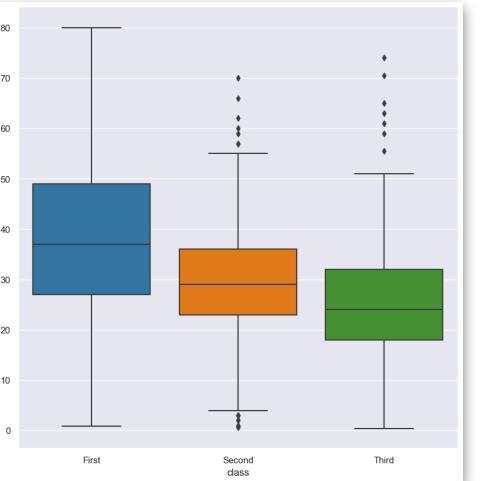
Purpose and philosophy

- **Fast, convenient and flexible** data analytics on the command line.
- Large input data sets are supported (> millions rows).
- Simple tasks should be simple. Complex tasks should be possible.
 - Highly customisable, but sensible defaults used extensively.

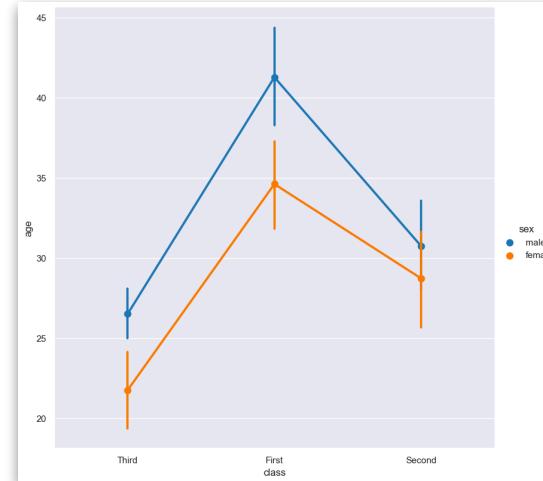
Supported basic plot types



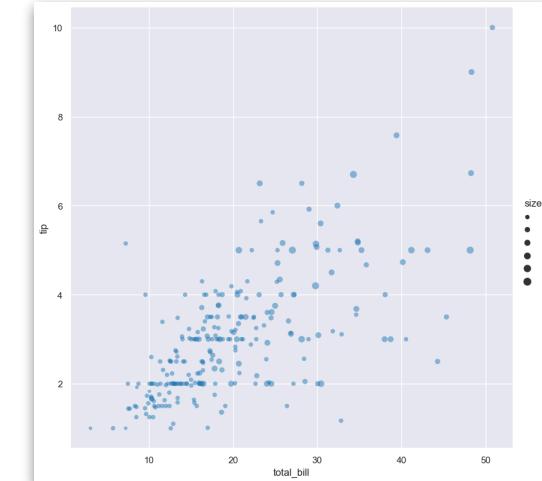
histogram



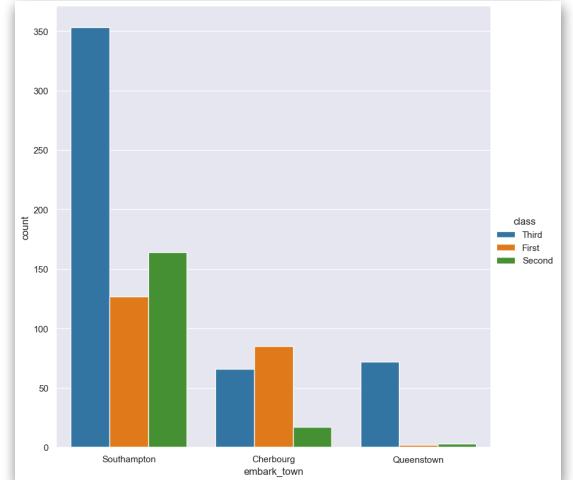
box



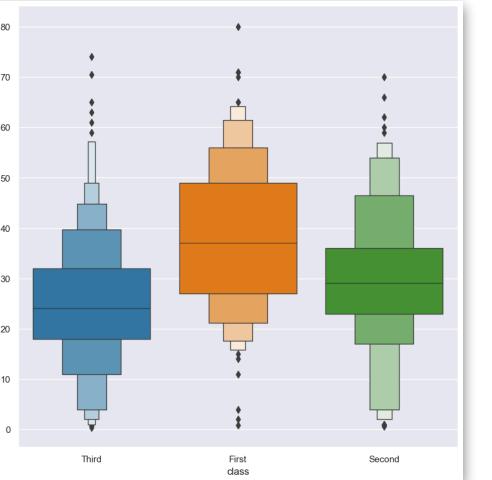
point



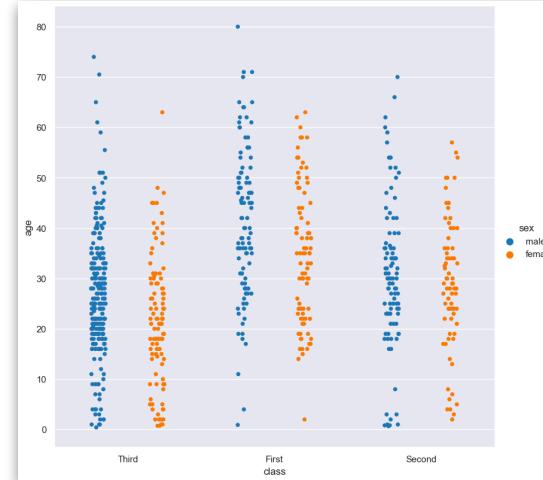
scatter



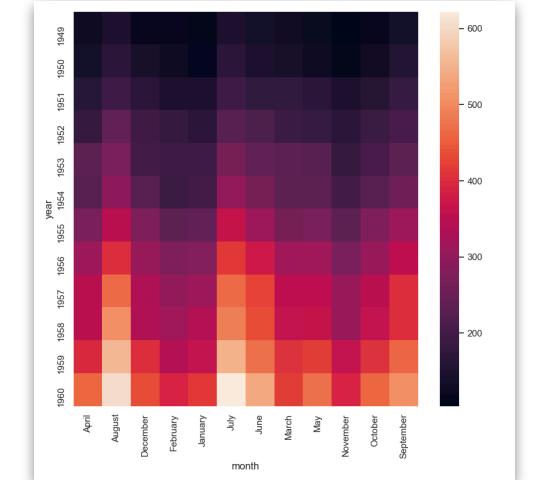
count



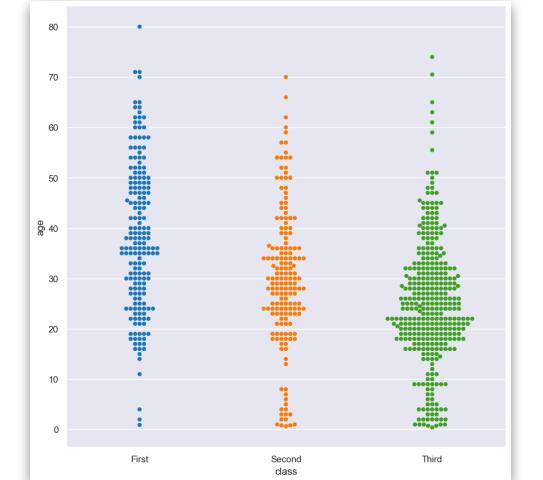
boxen



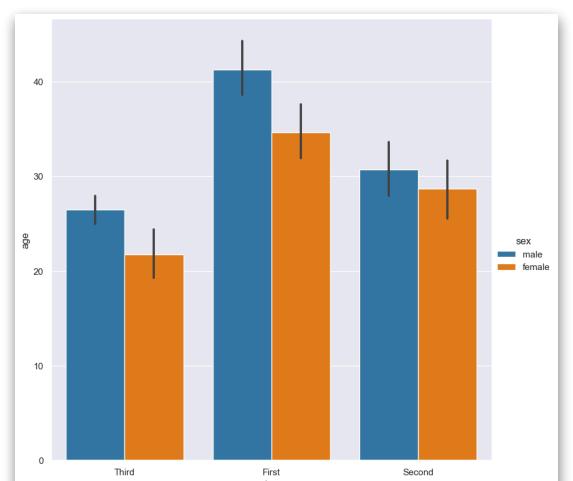
strip



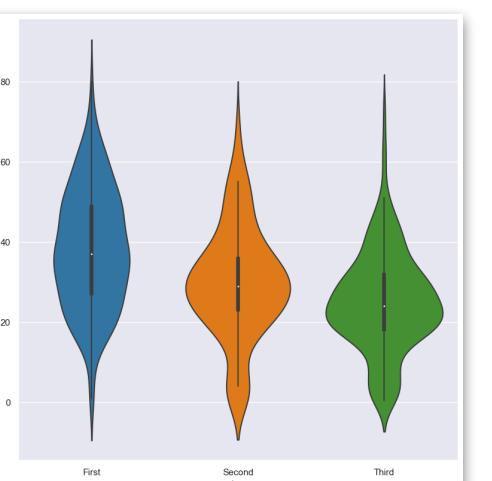
heat map



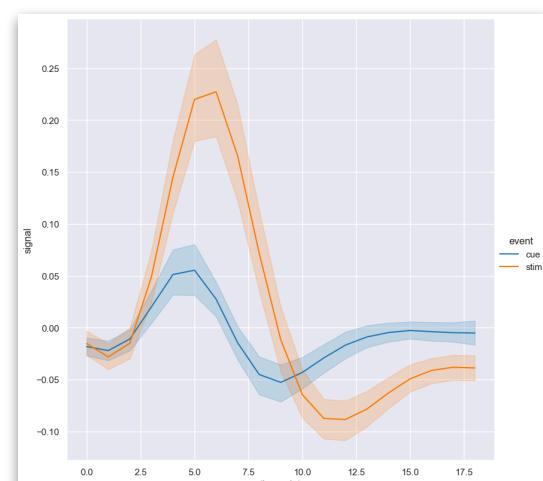
swarm



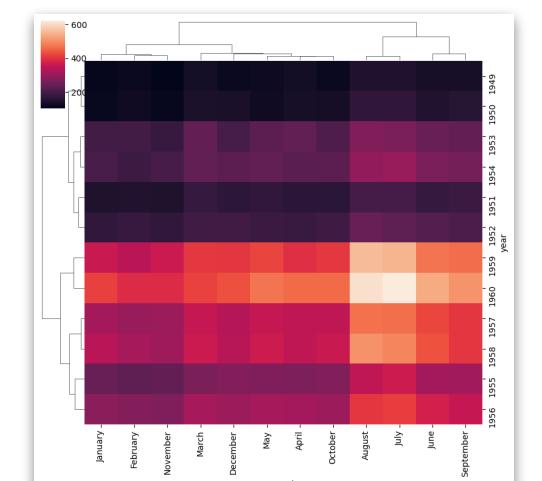
bar



violin



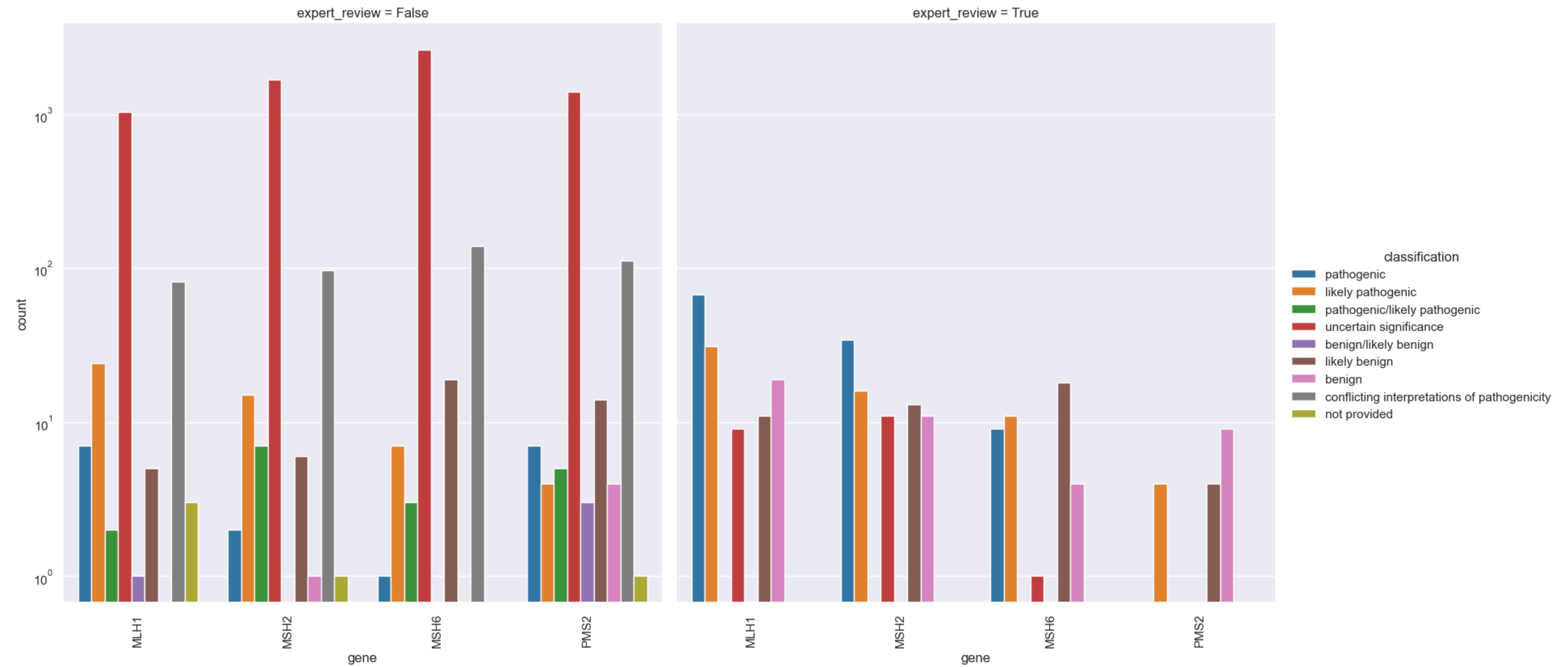
line



cluster map

Facets

```
cat mmr.csv | hatch count -x gene --hue classification --col expert_review
```



Supported data transformations

name	description
<u>corr</u>	pairwise correlation
<u>cut</u>	column selection
eval	compute new columns from existing data
filter	filter rows using a logical expression
<u>gmm</u>	Gaussian mixture model clustering
<u>head</u>	select the first N rows in the data
<u>kmeans</u>	k-means clustering
<u>melt</u>	reshape wide format into long format
pca	principal component analysis
<u>pivot</u>	reshape long format into wide format
sample	randomly sample rows
<u>sort</u>	sort rows
<u>tail</u>	select the last N rows in the data

underline = new since last version of hatch

Limitations of previous version

- Only one plot per command.
- `filter`, `eval`, `sample` done in predefined order, and only once per invocation of `hatch`.
- **Not modular.**
 - For example: PCA plot might involve pca-transformation, clustering, and a scatter plot.
 - Previously these were all bundled together in one command.
 - Each part ought to be usable on its own.
 - No way to combine parts in novel ways.
- Inadequate documentation.
- No logo!

Addressing the most important problem first



clearly I'm not a
graphic artist

Modularity brainwave

- Make each basic task its own command.
- Allow commands to be chained together.
- Data flows left to right in the chain.

how to express
this on the
command line?

Syntax for command chain

hatch command₁ + command₂ + . . . + command_n

Syntax for command chain

hatch command₁ + command₂ + . . . + command_n

multiple commands are
separated by +

Syntax for command chain



`hatch command1 + command2 + ... + commandn`

data flows from left to right
and may be transformed
along the way

Syntax for command chain

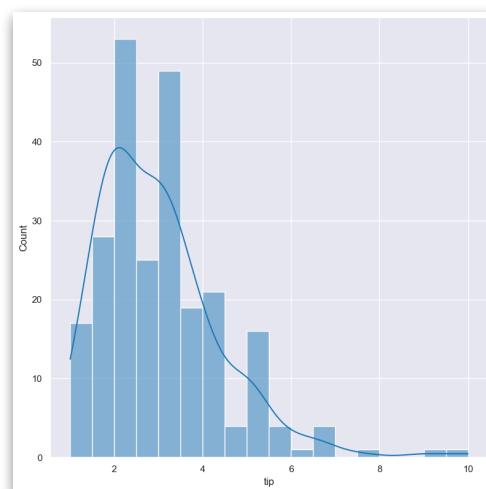
hatch command₁ + histogram + . . . + command_n

plot commands
generate images



plot commands
pass data on
unchanged

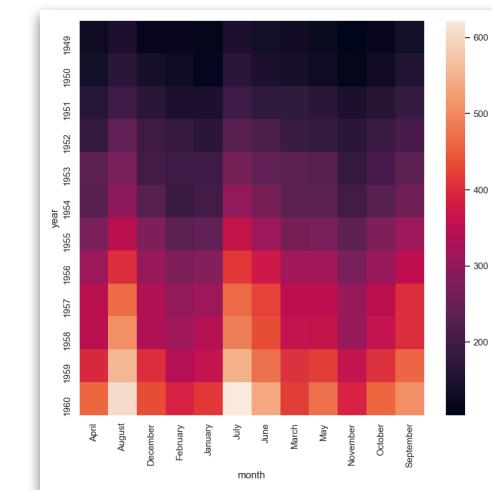
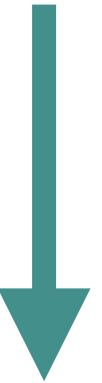
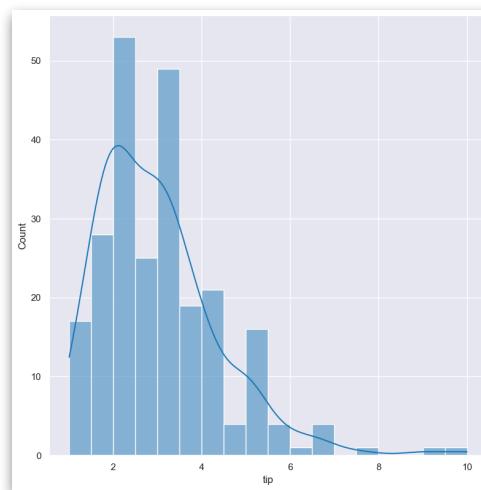
image



Syntax for command chain

complex chains can be formed
and multiple plots are possible

hatch command₁ + plot₁ + command₂ + plot₂ + . . .



Commands have optional arguments

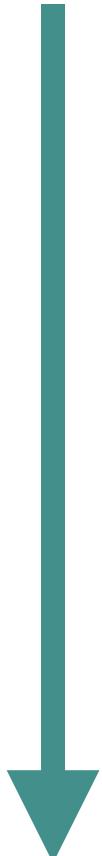
```
hatch command1 [ args ] + . . . + commandn [ args ]
```

Standard input

if the first command is
not an explicit input
command hatch inserts
an implicit `stdin` at the
start of the chain

`hatch tail`

equivalent* to

 `hatch stdin + tail`

* see next slide for full transformation of this command

Standard output

if the last command is a data transformation then hatch inserts an implicit `stdout` at the end of the chain

`hatch tail`

really equivalent to

`hatch stdin + tail + stdout`

Standard input and output

`stdin*` and `stdout` are commands that read / write data from the standard input / output device in CSV format by default. You can specify explicitly with `--format` argument.

`hatch tail`

really equivalent to

`hatch stdin + tail + stdout`

* `stdin` may only be used at most once and only as the first command

Named input and output files

hatch in iris.csv + tail

there is an implicit + stdout at
the end of this chain

in is a command that reads data from a named file. The format is guessed from the extension but you can specify explicitly with --format

Named input and output files

```
hatch tail + out new.tsv
```

there is an implicit `stdin` + at
the start of this chain

out is a command that writes data to a named file. The format is guessed from the extension but you can specify explicitly with `--format`

Named input and output files

hatch in iris.csv + tail + out new.csv

no implicit stdin or stdout here

Data transformation example

```
cat iris.csv | hatch sort -c sepal_length + tail 10  
sepal_length,sepal_width,petal_length,petal_width,species  
7.2,3.2,6.0,1.8,virginica  
7.2,3.6,6.1,2.5,virginica  
7.3,2.9,6.3,1.8,virginica  
7.4,2.8,6.1,1.9,virginica  
7.6,3.0,6.6,2.1,virginica  
7.7,2.8,6.7,2.0,virginica  
7.7,2.6,6.9,2.3,virginica  
7.7,3.8,6.7,2.2,virginica  
7.7,3.0,6.1,2.3,virginica  
7.9,3.8,6.4,2.0,virginica
```

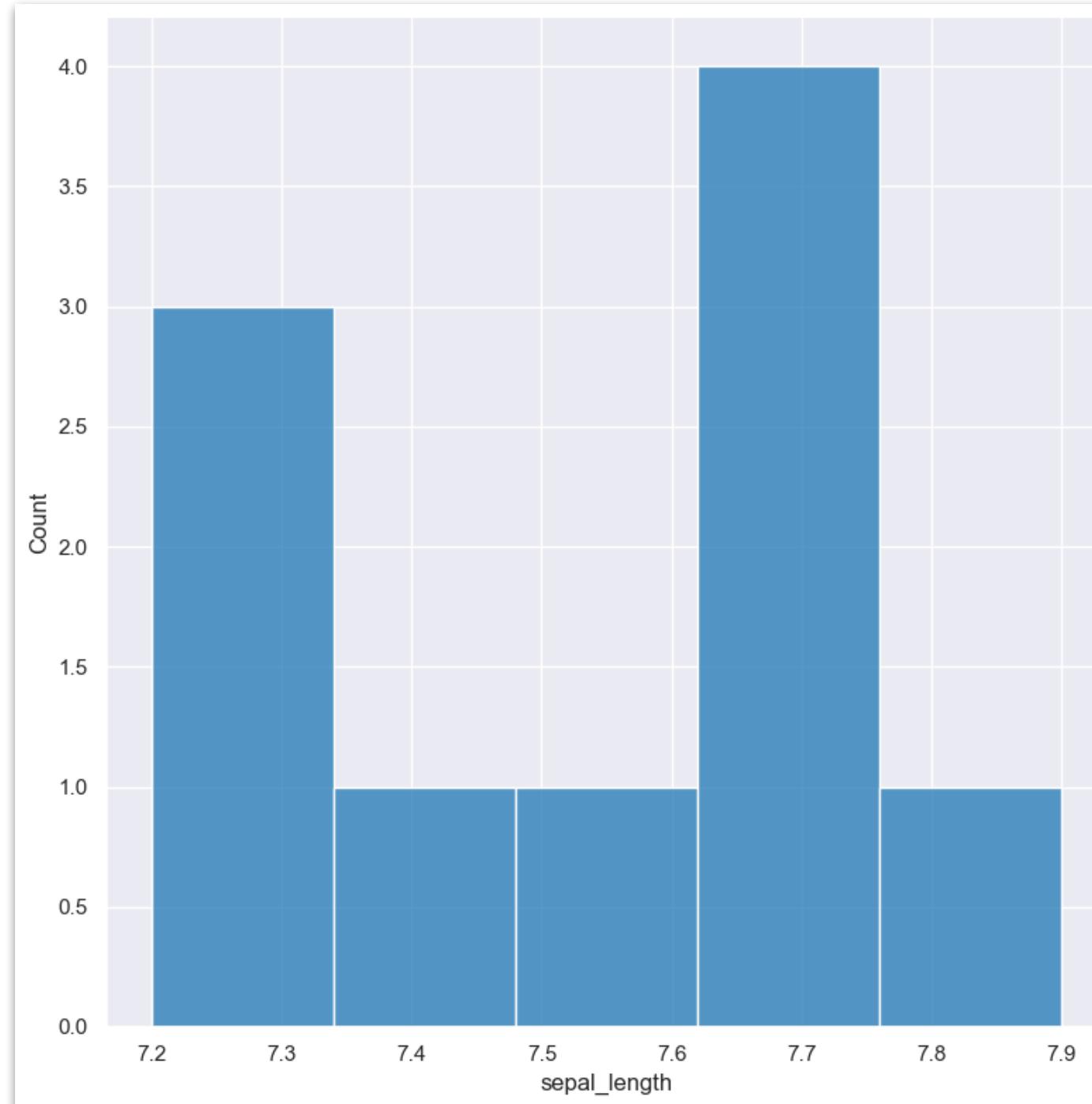
Data transformation example

```
cat iris.csv | hatch sort -c sepal_length + tail 10  
sepal_length,sepal_width,petal_length,petal_width,species  
7.2,3.2,6.0,1.8,virginica  
7.2,3.6,6.1,2.5,virginica  
7.3,2.9,6.3,1.8,virginica  
7.4,2.8,6.1,1.9,virginica  
7.6,3.0,6.6,2.1,virginica  
7.7,2.8,6.7,2.0,virginica  
7.7,2.6,6.9,2.3,virginica  
7.7,3.8,6.7,2.2,virginica  
7.7,3.0,6.1,2.3,virginica  
7.9,3.8,6.4,2.0,virginica
```

input is read from `stdin`,
then sorted (ascending) on the
`sepal_length` column, then
the last 10 rows are selected
and output to `stdout`

Data transformation and plotting example

```
cat iris.csv | hatch sort -c sepal_length + tail 10 + histogram -x sepal_length
```

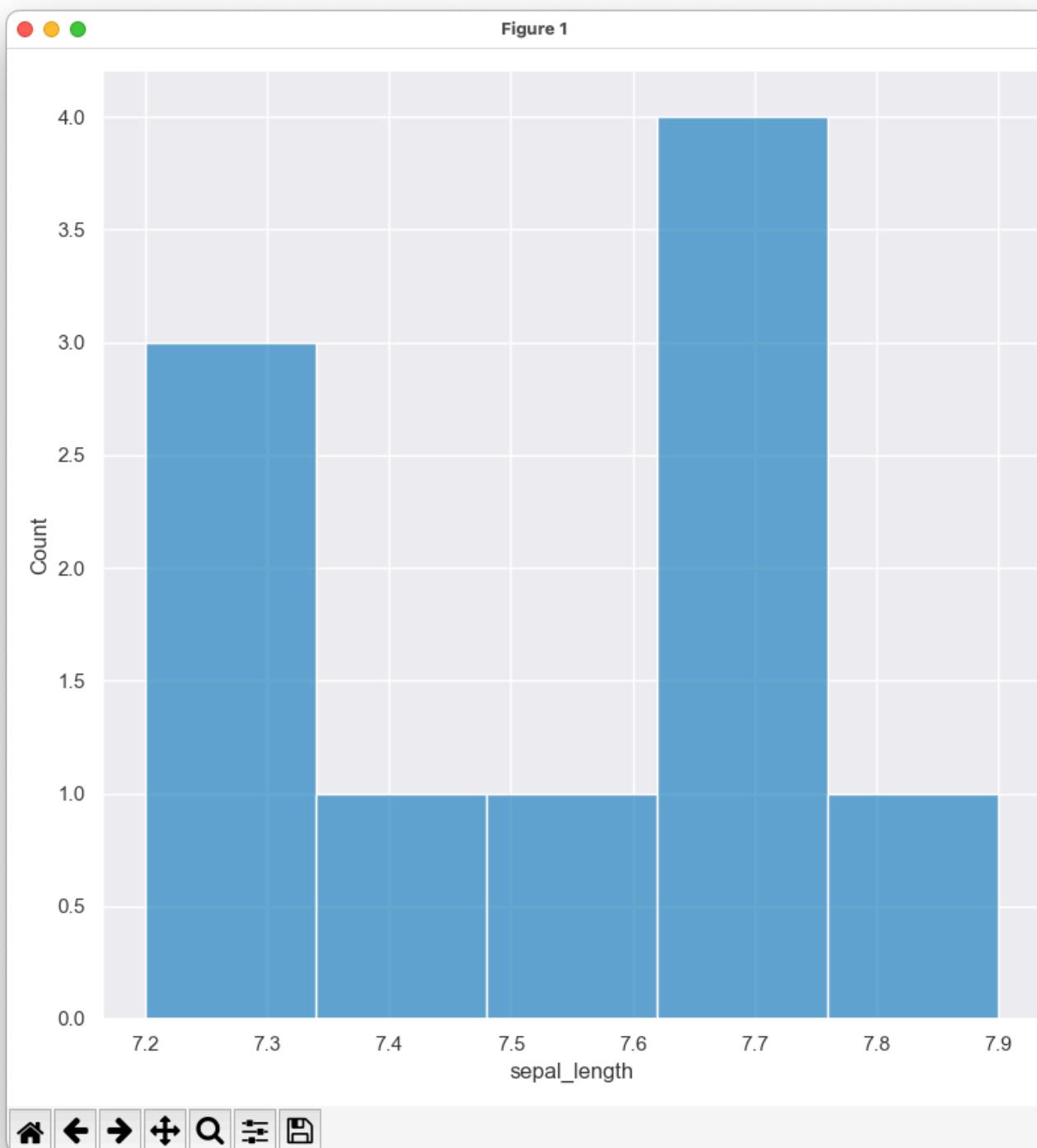


output is written to
hatch.sepal_length.histogram.png

*nothing is printed on
stdout because the last
command is a plot

Data transformation and interactive plotting example

```
cat iris.csv | hatch sort -c sepal_length + tail 10 + histogram -x sepal_length --show
```



An interactive window displays the current plot, no file is generated.

PCA example

```
cat iris.csv | hatch pca + pretty
```

sepal_length	sepal_width	petal_length	petal_width	species	pc1	pc2
5.1	3.5	1.4	0.2	setosa	-2.264542	0.505704
4.9	3.0	1.4	0.2	setosa	-2.086426	-0.655405
4.7	3.2	1.3	0.2	setosa	-2.367950	-0.318477
4.6	3.1	1.5	0.2	setosa	-2.304197	-0.575368
5.0	3.6	1.4	0.2	setosa	-2.388777	0.674767
...
6.7	3.0	5.2	2.3	virginica	1.870522	0.382822
6.3	2.5	5.0	1.9	virginica	1.558492	-0.905314
6.5	3.0	5.2	2.0	virginica	1.520845	0.266795
6.2	3.4	5.4	2.3	virginica	1.376391	1.016362
5.9	3.0	5.1	1.8	virginica	0.959299	-0.022284

[150 rows x 7 columns]

PCA example

```
cat iris.csv | hatch pca + pretty
```

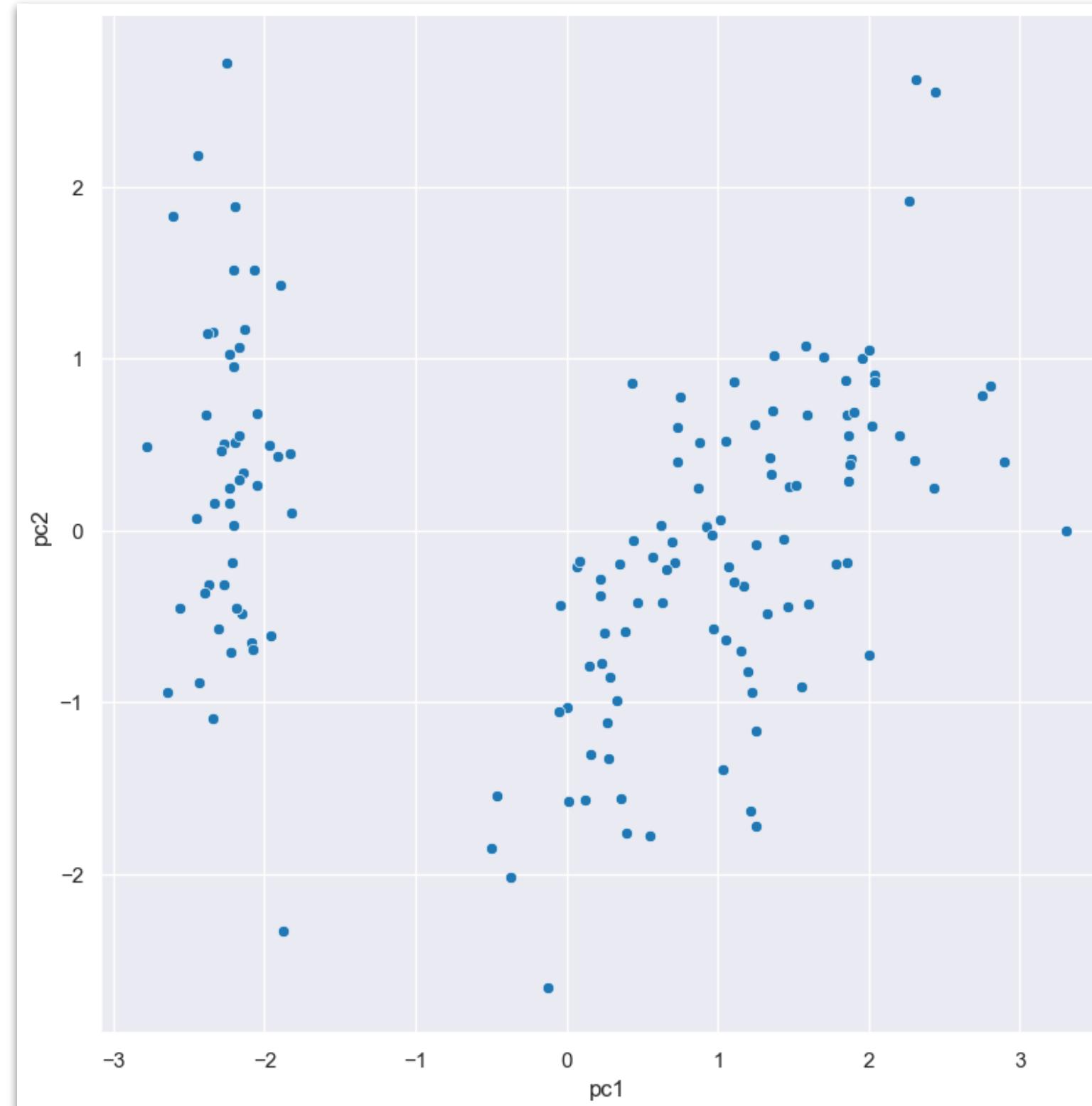
sepal_length	sepal_width	petal_length	petal_width	species	pc1	pc2
5.0	3.6	1.4	0.2	setosa	-2.264542	0.505704
...	setosa	-2.086426	-0.655405
6.7	3.0	5.2	2.3	virginica	1.870522	0.382822
6.3	2.5	5.0	1.9	virginica	1.558492	-0.905314
6.5	3.0	5.2	2.0	virginica	1.520845	0.266795
6.2	3.4	5.4	2.3	virginica	1.376391	1.016362
5.9	3.0	5.1	1.8	virginica	0.959299	-0.022284

[150 rows x 7 columns]

in this case 2 extra columns (pc1, pc2) are added to the data

PCA example with scatter plot

```
cat iris.csv | hatch pca + scatter -x pc1 -y pc2
```



output is written to
hatch.pc1.pc2.scatter.png

note that the scatter
command refers to the new
pc1 and pc2 columns

PCA example with k-means clustering

```
cat iris.csv | hatch pca + kmeans -n 2 -c pc1 pc2 + pretty
```

sepal_length	sepal_width	petal_length	petal_width	species	pc1	pc2	cluster
5.1	3.5	1.4	0.2	setosa	-2.264542	0.505704	0
4.9	3.0	1.4	0.2	setosa	-2.086426	-0.655405	0
4.7	3.2	1.3	0.2	setosa	-2.367950	-0.318477	0
4.6	3.1	1.5	0.2	setosa	-2.304197	-0.575368	0
5.0	3.6	1.4	0.2	setosa	-2.388777	0.674767	0
...
6.7	3.0	5.2	2.3	virginica	1.870522	0.382822	1
6.3	2.5	5.0	1.9	virginica	1.558492	-0.905314	1
6.5	3.0	5.2	2.0	virginica	1.520845	0.266795	1
6.2	3.4	5.4	2.3	virginica	1.376391	1.016362	1
5.9	3.0	5.1	1.8	virginica	0.959299	-0.022284	1

[150 rows x 8 columns]

PCA example with k-means clustering

```
cat iris.csv | hatch pca + kmeans -n 2 -c pc1 pc2 + pretty
```

use kmeans to find 2 clusters in the data using
only the columns pc1 and pc2

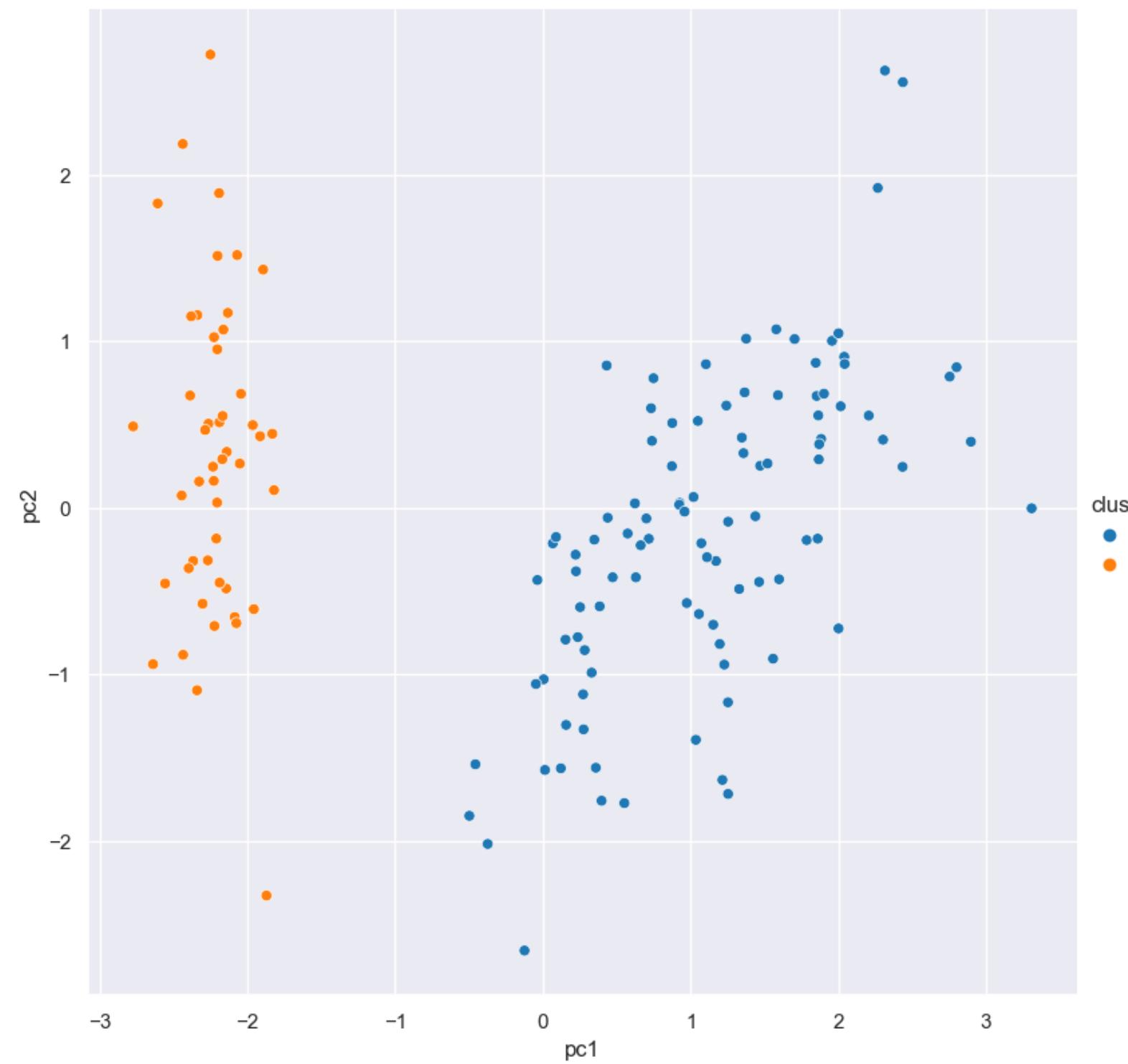
			width	species	pc1	pc2	cluster
4.7	3.2	1.3	0.2	setosa	-2.264542	0.505704	0
4.6	3.1	1.5	0.2	setosa	-2.086426	-0.655405	0
5.0	3.6	1.4	0.2	setosa	-2.367950	-0.318477	0
5.4	3.9	1.7	0.2	setosa	-2.304197	-0.575368	0
5.0	3.4	1.4	0.2	setosa	-2.388777	0.674767	0
...
6.7	3.0	5.2	2.3	virginica	1.870522	0.382822	1
6.3	2.5	5.0	1.9	virginica	1.558492	-0.905314	1
6.5	3.0	5.2	2.0	virginica	1.520845	0.266795	1
6.2	3.4	5.4	2.3	virginica	1.376391	1.016362	1
5.9	3.0	5.1	1.8	virginica	0.959299	-0.022284	1

[150 rows x 8 columns]

1 extra column (**cluster**) is added to the data

PCA example with k-means clustering and scatter plot

```
cat iris.csv | hatch pca + kmeans -n 2 -c pc1 pc2 + scatter -x pc1 -y pc2 --hue cluster
```



output is written to
hatch.pc1.pc2.cluster.scatter.png

note that the scatter
command refers to the new
cluster column

Bioinformatics example: copy number analysis

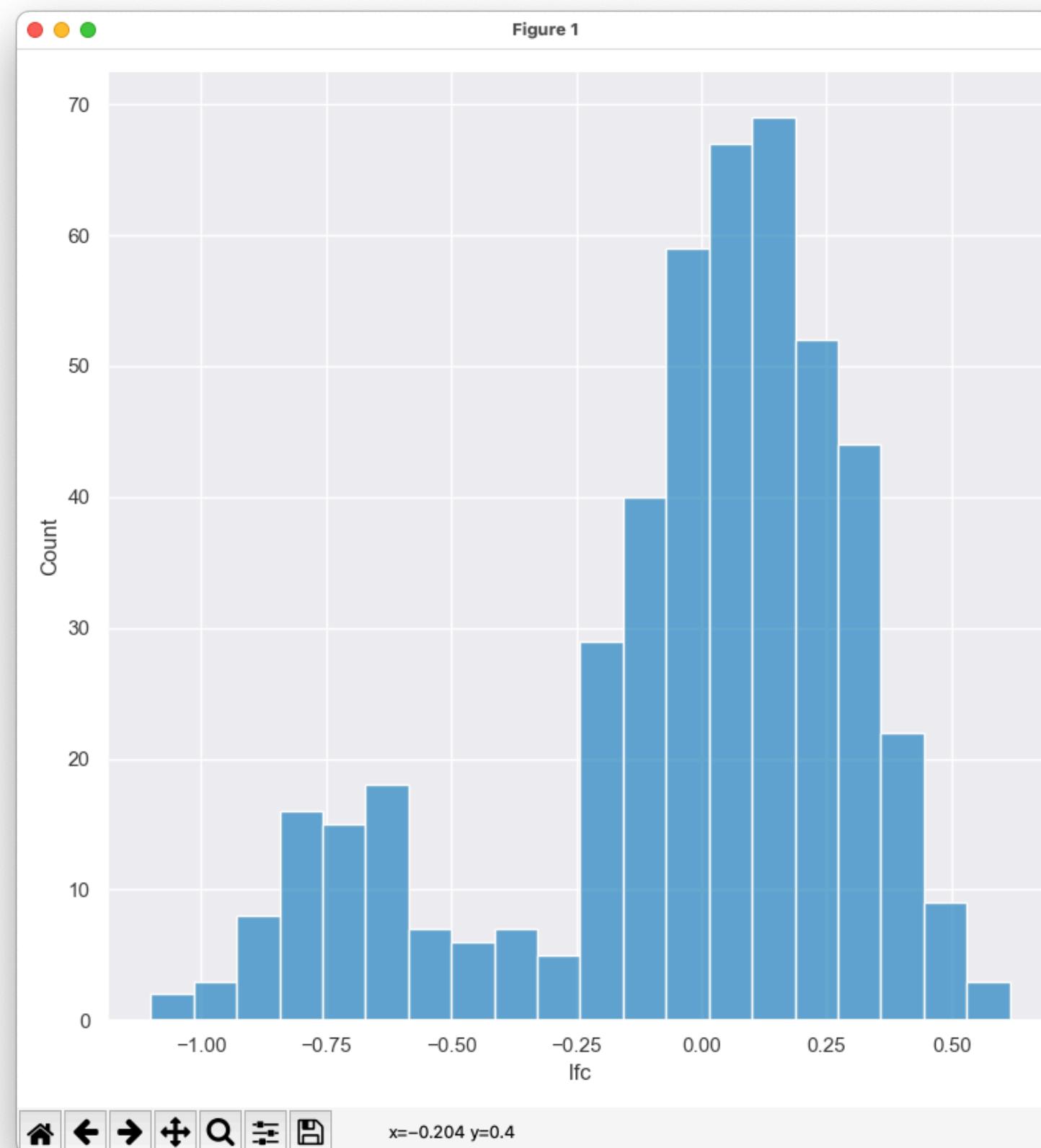
```
cat TSO500.lfc.csv | hatch pretty -c chrom start end gene lfc gene_ordinal sample_code
```

chrom	start	end	gene	lfc	gene_ordinal	sample_code
chr1	8013207.0	8025060.0	ERRFI1	0.391513	0	A1
chr1	9710453.0	9727048.0	PIK3CD	-0.215299	1	A1
chr1	11107482.0	11259411.0	MTOR	-0.135017	2	A1
chr1	15848065.0	15939429.0	SPEN	0.210534	3	A1
...
chr22	28687894.0	28741491.0	CHEK2	-0.385767	483	J9
chr22	29268006.0	29300527.0	EWSR1	-0.382720	484	J9
chr22	29603996.0	29694804.0	NF2	-0.109701	485	J9
chr22	37973492.0	37983786.0	SOX10	-0.922735	486	J9
chr22	41093002.0	41178958.0	EP300	0.180778	487	J9

[24023 rows x 27 columns]

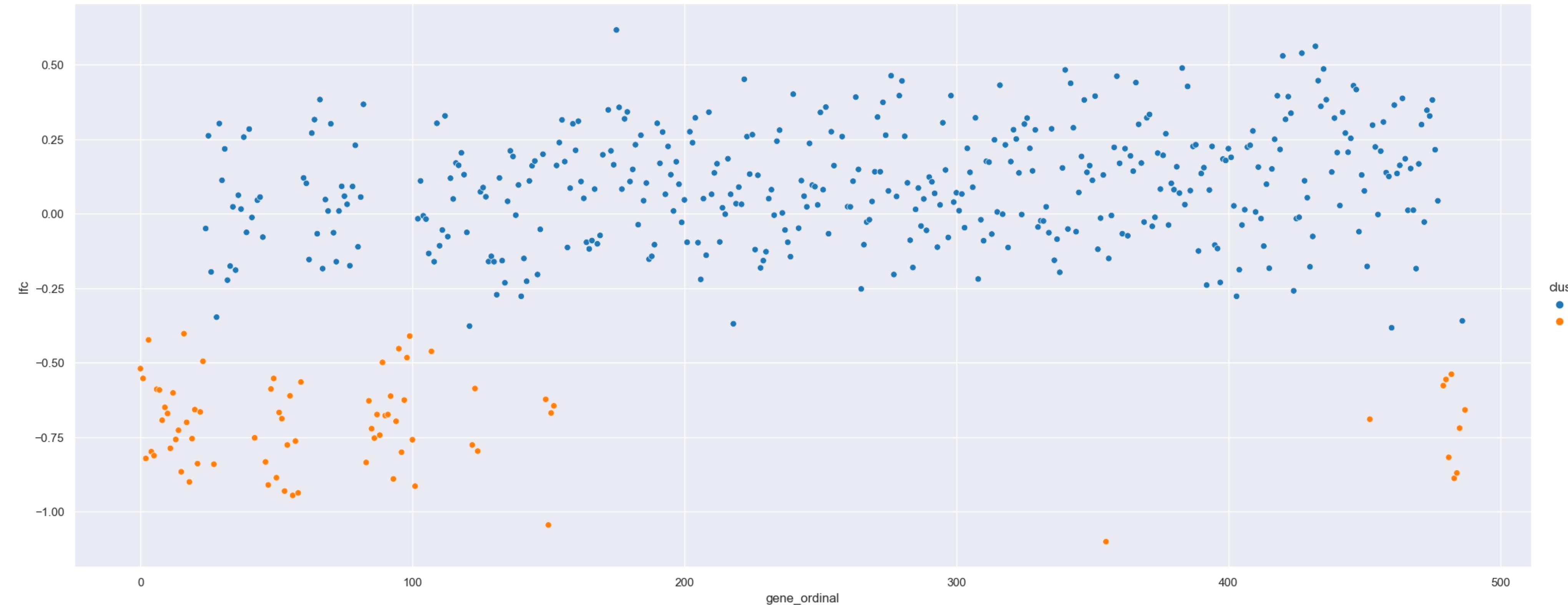
Bioinformatics example: copy number analysis

```
cat TSO500.lfc.csv | hatch filter 'sample_code == "B1"' + histogram -x lfc --show
```



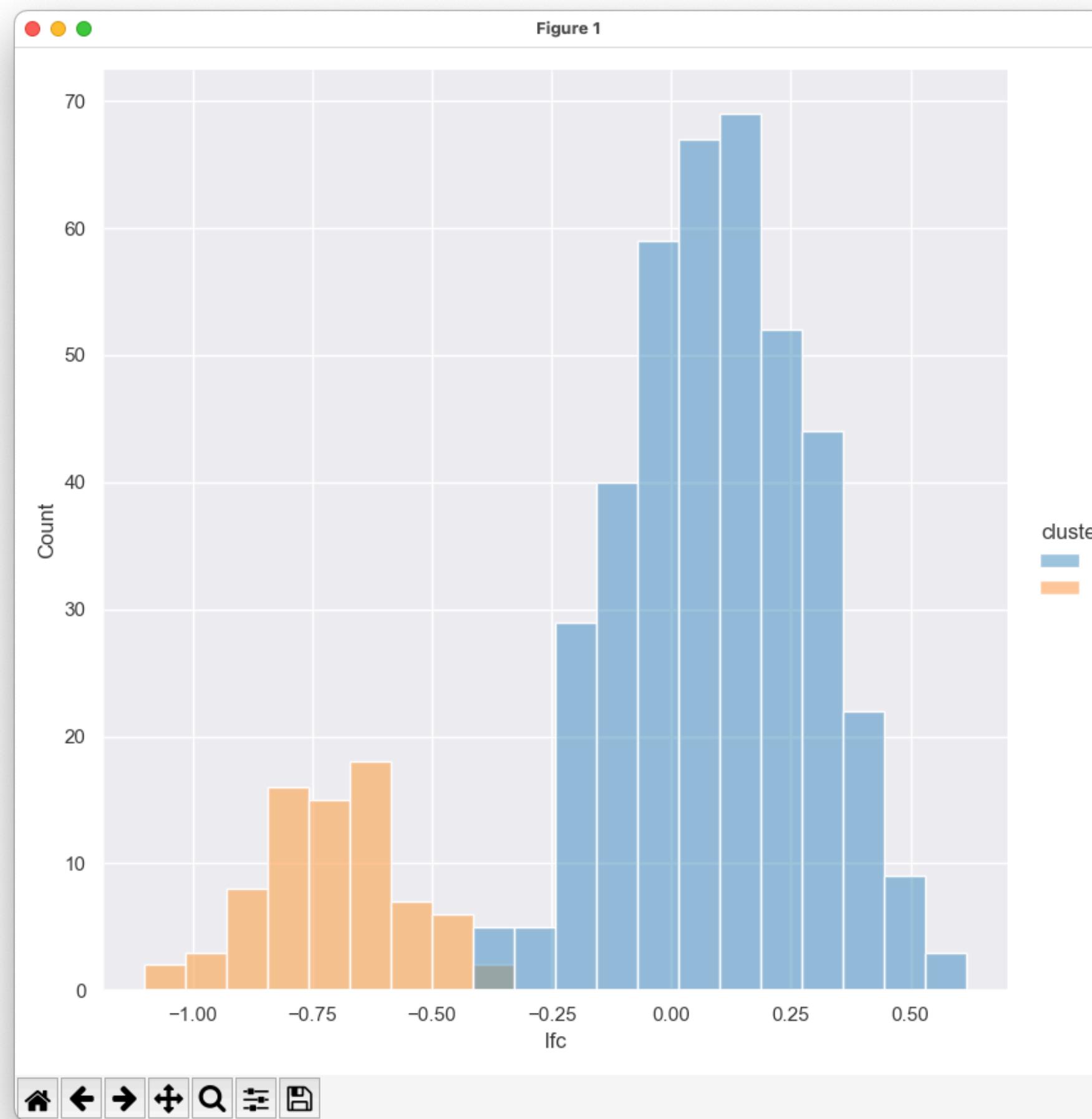
Bioinformatics example: copy number analysis

```
cat TSO500.lfc.csv | hatch filter 'sample_code == "B1"' + \
gmm -n 2 -c lfc + \
scatter -x gene_ordinal -y lfc --hue cluster --width 20
```



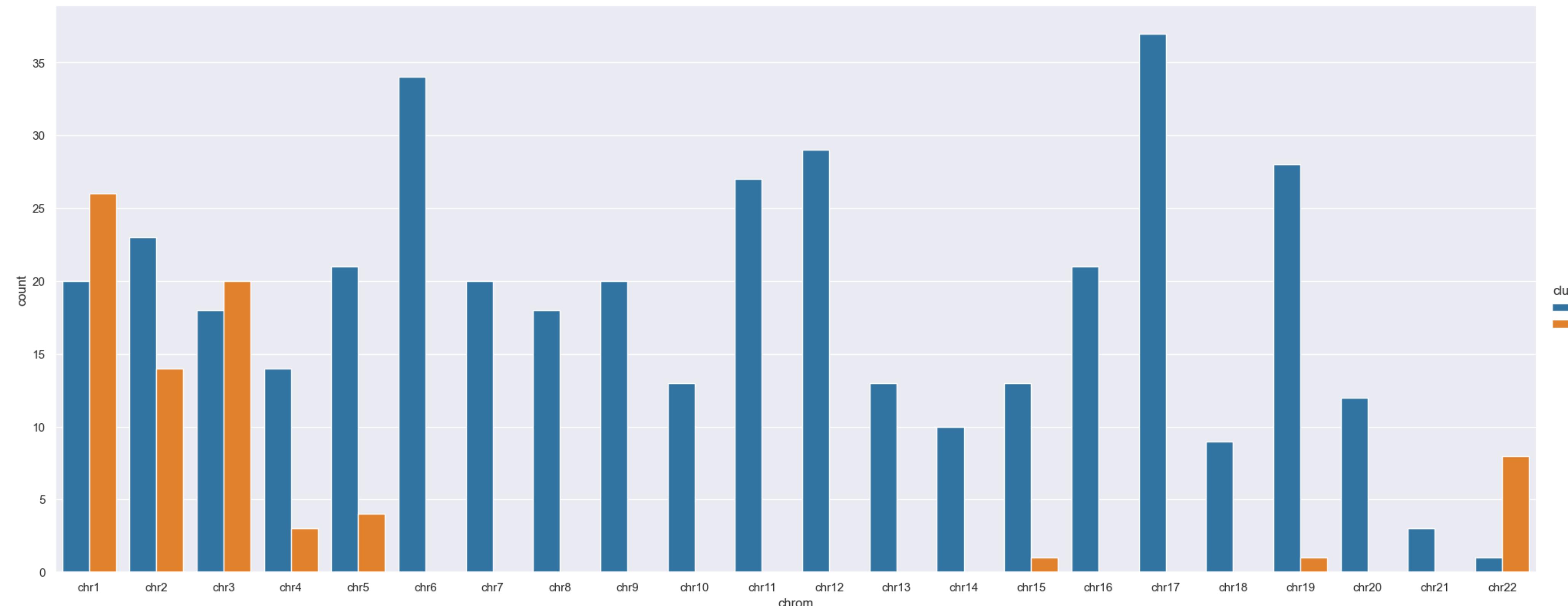
Bioinformatics example: copy number analysis

```
cat TS0500.lfc.csv | hatch filter 'sample_code == "B1"' + gmm -n 2 -c lfc + histogram -x lfc --hue cluster --show
```



Bioinformatics example: copy number analysis

```
cat TSO500.lfc.csv | hatch filter 'sample_code == "B1"' + \  
gmm -n 2 -c lfc + \  
count -x chrom --hue cluster --width 20
```



Code and documentation

- code:
github.com/bjpop/hatch
- documentation:
hatch.readthedocs.io

TODO

- More testing of the code.
- Complete the documentation.
- More useful plots and transformations.
- Beg people to use it.
- Try to publish.