

Global-Sigma

immediate

August 30, 2017

Contents

1 Gaussian kernel width sigma	1
Using <code>find_sigmas</code>	1

1 Gaussian kernel width sigma

The other important parameter for `DiffusionMap` is the Gaussian kernel width `sigma` (σ) that determines the transition probability between data points. The default call of **destiny** – `DiffusionMap(data)` aka `DiffusionMap(data, 'local')` – uses a local `sigma` per cell, derived from a local density estimate around each cell.

Using the 1.0 default, `sigma = 'global'`, estimates `sigma` using a heuristic. It is also possible to specify this parameter manually to tweak the result. The eigenvector plot explained above will show a continuous decline instead of sharp drops if either the dataset is too big or the `sigma` is chosen too small.

The `sigma` estimation algorithm is explained in detail in [Haghverdi et al. \(2015\)](#). In brief, it works by finding a maximum in the slope of the log-log plot of local density versus `sigma`.

```
In [2]: library(destiny)
        data(guo_norm)
```

Using `find_sigmas`

An efficient variant of that procedure is provided by `find_sigmas`. This function determines the optimal `sigma` for a subset of the given data and provides the default `sigma` for a `DiffusionMap` call. Due to a different starting point, the resulting `sigma` is different from above:

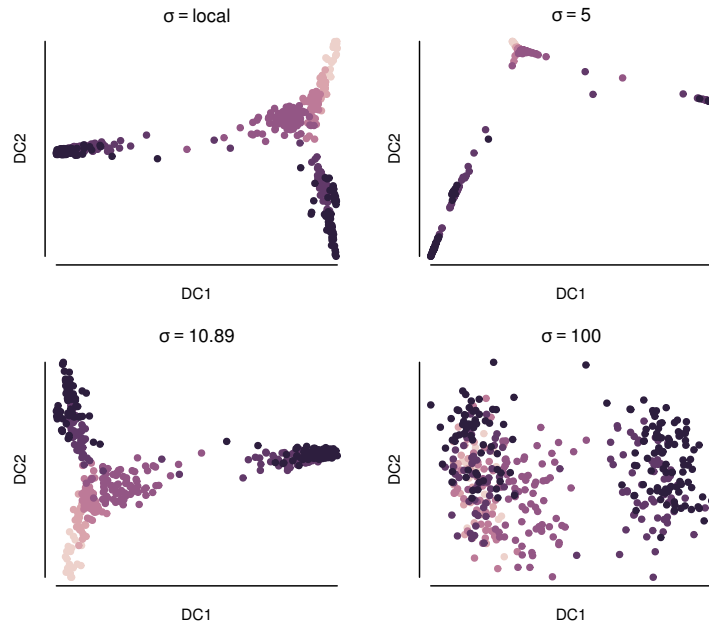
```
In [3]: sigmas <- find_sigmas(guo_norm, verbose = FALSE)
        optimal_sigma(sigmas)
```

```
10.8945955274194
```

The resulting diffusion map's approximation depends on the chosen `sigma`. Note that the `sigma` estimation heuristic only finds local optima and even the global optimum of the heuristic might not be ideal for your data.

```
In [4]: par(pch = 20, mfrow = c(2, 2), mar = c(3,2,2,2))
        palette(cube_helix(6))

        for (sigma in list('local', 5, round(optimal_sigma(sigmas), 2), 100))
          plot(DiffusionMap(guo_norm, sigma), 1:2,
               main = substitute(sigma == s, list(s = sigma)),
               col_by = 'num_cells', draw_legend = FALSE)
```



References

Haghverdi, L., F. Buettner, and F. J. Theis
 2015. Diffusion maps for high-dimensional single-cell analysis of differentiation data. *Bioinformatics*, (in revision).