

Global-Sigma

immediate

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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`.

```
[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:

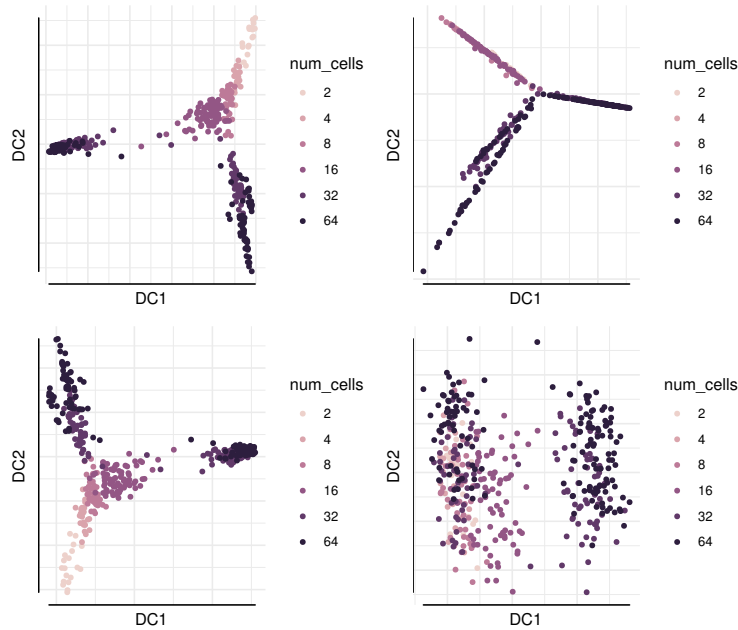
```
[3]: sigmas <- find_sigmas(guo_norm, verbose = FALSE)
      optimal_sigma(sigmas)
```

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.

```
[4]: palette(cube_helix(6))

plots <- lapply(
  list('local', 5, round(optimal_sigma(sigmas), 2), 100),
  function(sigma) plot(
    DiffusionMap(guo_norm, sigma), 1:2,
    main = paste('σ =', sigma),
    col_by = 'num_cells', draw_legend = FALSE))
do.call(gridExtra::grid.arrange, c(plots, ncol = 2))
```



References

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