Test script for olfactory receptors of Drosophila are sensitive to molecular volume of odorants

April 15, 2015

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This simple code provided to test volume sensitivity of Olfactory Receptors. At first, we extract molecular volumes and responses from supplementary data.

```
> DoOR <- as.matrix( read.csv("proposed_odorants.csv") )
> rownames( DoOR ) <- DoOR[, 1]
> DoOR <- DoOR[, 2:33]
> mode( DoOR ) <- "numeric"
```

DoOR represents response of odor receptors(columns) to odorants(rows), for example:

```
> DoOR[ 1:5 , 1:5 ]
```

	Or10a	Or1a	Or22a	Or22b	Or23a
7732-18-5	NA	0.024878414	NA	NA	NA
7664-41-7	0.06296634	NA	0.10187126	NA	NA
124-38-9	0.05848141	0.007108118	0.06253786	0	0.023889161
67-56-1	0.05113509	NA	0.11791586	NA	0.013155924
64-18-6	0.12837361	NA	0.05348513	NA	0.002192654

```
> odorants <- as.matrix( read.csv("odorants.csv") )
> volume <- as.numeric( odorants[, 4] )
> names( volume ) <- odorants[, 1]
```
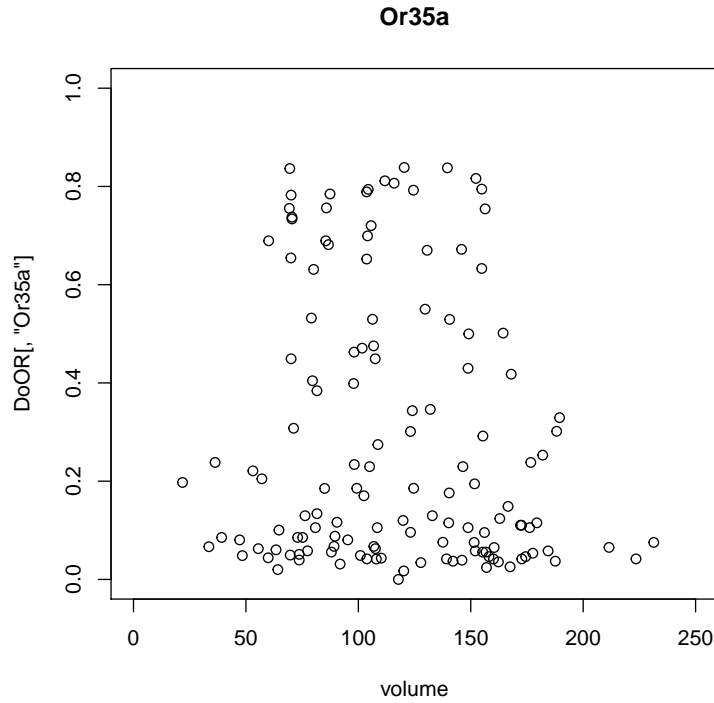
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We also have vector of molecular volumes:

```
> volume[1:10]
```

```
7732-18-5 7664-41-7  124-38-9   67-56-1   64-18-6   75-07-0   79-09-4   64-17-5
     19.8      21.8      33.5      36.3      39.2      47.2      48.4      53.1
  64-19-7  124-40-3
     55.5      57.1
```

We can plot response of ORs versus molecular volumes for every receptors:

```
> plot(volume, DoOR[ ,"Or35a" ], ylim=c(0,1), xlim=c(0,250), main="Or35a" )
```


to find out how odor receptors are sensitive to molecular volume of odorants we try to obtain $f_n(v)$, which express prefered volume(v_n) and flexibility(σ_n) of binding packets:

$$f_n(v) = e^{-\frac{(v-v_n)^2}{2\sigma_n^2}} , \qquad (1)$$

$$\frac{1}{\sigma_n^2} = \frac{1}{\sigma_{h_n}^2} - \frac{1}{\sigma_{g_n}^2} \qquad (2)$$

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$$v_n = \sigma_n^2 \left(\frac{\mu_{h_n}}{\sigma_{h_n}^2} - \frac{v_{g_n}}{\sigma_{g_n}^2} \right). \tag{3}$$

where μ_{h_n} and σ_{h_n} are:

$$\frac{1}{\sigma_n^2} = \frac{1}{\sigma_{h_n}^2} - \frac{1}{\sigma_{g_n}^2} \tag{4}$$

$$\frac{v_n}{\sigma_n^2} = \frac{\mu_{h_n}}{\sigma_{h_n}^2} - \frac{v_{g_n}}{\sigma_{g_n}^2}. \tag{5}$$

required functions is defined as following:

```
> wt.mean <- function (x, wt)                    #Weighted mean function
+   {
+     s = which(!is.na(x * wt))
+     wt = wt[s]
+     x = x[s]
+     return(sum(wt * x)/sum(wt))
+   }
> wt.sd <- function (x, wt)                       #Weighted sd function
+   {
+     s = which(!is.na(x + wt))
+     wt = wt[s]
+     x = x[s]
+     xbar = wt.mean(x, wt)
+     return(sqrt( sum(wt * (x^2))/sum(wt) - xbar^2)  )
+   }

> gauss <- function (x, mu=0, sig=1)             #Gaussian function
+   {
+     return( exp( -(x - mu)^2 / (2 * sig^2) ) )
+   }

> profile <- function(OR){
+     response = DoOR[, OR]                             #OR's response selection
+     sig_g = sd(volume, na.rm=T)                       #SD of g(v)
+     mu_g = mean(volume, na.rm=T)                      #MEAN of g(v)
+     sig_h = wt.sd(volume, response)                   #SD of h(v), 10th formula
+     mu_h =  wt.mean(volume, response)                 #MEAN of h(v), 9th formual
+
+     sig_f = sqrt( sig_g^2 * sig_h^2 / (sig_g^2 - sig_h^2) )     #SD of f(v)
+     mu_f = sig_f^2 * (mu_h/sig_h^2 - mu_g/sig_g^2)             #MEAN of f(v)
```

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```
+ return(c(mu_f, sig_f))
+ }
```

below we show receptors which their responses significantly are dependent to molecular volume and validated by bootstrapping test.

```
> colnames(DoOR)
```

```
 [1] "Or10a" "Or1a"  "Or22a" "Or22b" "Or23a" "Or24a" "Or2a"  "Or30a" "Or33a"
[10] "Or35a" "Or42a" "Or42b" "Or43a" "Or43b" "Or45b" "Or46a" "Or47a" "Or49a"
[19] "Or49b" "Or59a" "Or59b" "Or67a" "Or67b" "Or67c" "Or71a" "Or85a" "Or85b"
[28] "Or85c" "Or85f" "Or94b" "Or98a" "Or9a"
```

Everyone can choose one of them and see volume sensitivity of OR. Scatterplot shows response versus molecular volume and f(v) lines as volume dependancy or volume profile of OR.

```
>      OR = "Or35a"
>      para <- profile(OR)
>      mu_f <- para[1]
>      sig_f <- para[2]
>      f_v = gauss(volume, mu=mu_f, sig=sig_f)      #Making f(v) as a gaussian function
>      plot(volume, DoOR[ ,OR], ylim=c(0,1), xlim=c(0,250) , ylab="response"
+           , main=OR , col="blue" )
>      lines(volume,  f_v )
```

Or35a