Package: ionChannelData (via r-universe)

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Title Ion Channel Data for Hidden Markov Models

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Depends R (>= 3.5)

Description Data sets, from ion channel patch-clamp studies, to which hidden Markov models (based on the assumption of Gaussian distributed emissions) may be fitted.

Suggests eglhmm, depmixS4

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LazyData true

Repository https://rolfturner.r-universe.dev

RemoteUrl https://github.com/rolfTurner/ionChannelData

RemoteRef HEAD

RemoteSha 116952a6f533e8c51f8c45fd37be5fbdfc09255c

Contents

`ionChannelData` *Ion channel data*

Description

Time series of observations, made by means of patch clamps, of current in picoamps, across cell membranes.

Usage

```
ic25kHz_12_sgmnt1
ic25kHz_13_sgmnt2
ic25kHz_14_sgmnt2
ic25kHz_15_sgmnt2
ic50kHz_06_sgmnt2
ic50kHz_08_sgmnt2
ic50kHz_09_sgmnt1
ic50kHz_10_sgmnt1
```

Format

Data frames, each with a single numeric column named "current", with 200001, 200000, 200000, 200000, 199926, 200000 and 200000 observations respectively.

Details

Extensive high bandwidth patch clamp data were obtained in the laboratory of Professor Boris Martinac (Head of Mechanosensory Biophysics Laboratory, Victor Chang Cardiac Research Institute) from the MscL (large mechanosensitive ion channel) in the bacterium E. coli. The data were recorded by the same researcher in the same laboratory during the same afternoon under identical environmental conditions, with applied voltage +100 mV, bandwidths 25 kHz and 50 kHz and digitally sampled at 75 kHz and 150 kHz, respectively. Four recordings at each bandwidth were obtained, each containing between 5 and 30 million data values.

The data were screened and eight data sets (four at each bandwidth) each containing about 200,000 values were selected for analysis. This package contains these eight data sets.

Experimental technique: 6×His-tagged MscL proteins were purified, and the 6×His tag was removed by thrombin according to a published procedure (Häse et al. 1995). Purified MscL material was reconstituted into liposomes mixed with 100 % soybean azolectin using a dehydration/rehydration (D/R) reconstitution method (Delcour et al. 1989; Martinac et al. 2010). Mixed lipids were dissolved in chloroform and dried under nitrogen to make a thinner lipid film, and a D/R buffer [200 mM KCl, 5 mM 4-(2-hydroxyethyl)-1-piperazineethanesulphonic acid (HEPES), adjusted to pH 7.2 with KOH] was added before vortexing and sonication for 10 minutes. MscL was added at protein-to-lipid ratio of 1:1000 (w/w) and incubated at 4° C for 1 hour. Detergent was removed with the addition of Biobeads (BioRad, Hercules, CA), followed by incubation at 4° C for a further 3 hours. The proteoliposomes were collected by ultracentrifugation and resuspended in a 30 μ-litre D/R buffer. Aliquots of proteoliposomes were spotted onto cover slips and dehydrated overnight under vacuum at 4° C. The dried proteoliposomes were rehydrated at 4° C with a D/R buffer and subsequently used for electrophysiological experiments.

The MscL channel activity was recorded from proteoliposomes using the patch clamp technique at applied voltage +100 mV. The bath and pipette recording solution used in liposome experiments was the same, consisting of 200 mM KCl, 40 mM MgCl2 and 5 mM HEPES (pH 7.2 adjusted with KOH). Negative pressure (suction) activating MscL was applied to the patch pipette using a syringe, monitored with a pressure gauge (PM 015R, World Precision Instruments, Sarasota, FL). The single-channel current was amplified with an Axopatch 200B amplifier (Molecular Devices, Sunnyvale, CA), filtered at 25 and 50 kHz, digitized at 75 and 150 kHz, respectively, with a Digidata 1440A interface using pCLAMP 10 acquisition software (Molecular Devices, Sunnyvale, CA) and stored in a computer.

Note

These data are basically intended for use with the `eglhmm` package, as examples of data to which hidden Markov models with Gaussian emissions could be fitted. However their presence in the `eglhmm` package would cause the size of the `data` directory in that package to exceed 4.5 Mb., which is unacceptably large. Consequently these data sets have been placed in a separate "data only" package (the package currently under consideration). In the normal course of events, users will obtain this package (i.e. `ionChannelData`) from `github` via the commmand

```
install.packages("ionChannelData",repos="https://rolfturner.r-universe.dev")
```

Source

These data were obtained from the laboratory of Professor Boris Martinac, Victor Chang Cardiac Research Institute, Darlinghurst, Sydney, Australia.

References

Almanjahie, I. M.; Khan, R. N.; Milne, R. K.; Nomura, T; and Martinac, B. (2015). Hidden Markov analysis of improved bandwidth mechanosensitive ion channel data. *European Biophysics Journal* **44**, issue 7, pp. 545–556, DOI: https://doi.org/10.1007/s00249-015-1060-7.

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Häse, C. C.; Le Dain, A. C.; Martinac, B. (1995). Purification and functional reconstitution of the recombinant large mechanosensitive ion channel (MscL) of Escherichia coli. Journal of Biological Chemistry **270** pp. 18329–18334.

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Martinac, B.; Rohde, P. R.; Battle, A. R.; Petrov, P. P.; Foo; A. F.; Vásquez, V.; Huynh, T.; Kloda, A. (2010). Studying mechanosensitive ion channels using liposomes. In *Liposomes: Methods and Protocols, Volume 2: Biological Membrane Models*, Volkmar Weissig ed., *Springer* book series *Methods in Molecular Biology* **606**, pp. 31–53.

Examples

```
if(requireNamespace("eglhmm")) {
    # Extract tiny subset, to run fast.
    X    <- ionChannelData::ic25kHz_12_sgmnt1[1:1000,1,drop=FALSE]
    fit0 <- eglhmm::eglhmm(current ~ 1,data=X,distr="Gaussian",K=7,
                   method="em",tolerance=1e-6,verb=TRUE,itmax=1500)
    fit1 <- eglhmm::eglhmm(current ~ 1,data=X,distr="Gaussian",K=7,
                           preSpecSigma=seq(0.5,3.5,length=7),
                           method="em",tolerance=1e-6,verb=TRUE,
                           itmax=1500)
```

```
}
## Not run:  # Takes a VERY long time.  Total of 645 (slow!) EM steps.
    if(requireNamespace("eglhmm")) {
        X    <- ic25kHz_12_sgmnt1
        fit2 <- eglhmm::eglhmm(current ~ 1,data=X,distr="Gaussian",K=7,
                method="em",tolerance=1e-6,verb=TRUE,itmax=1000)
# Compare results from depmixS4.
        if(requireNamespace("depmixS4")) {
            mdl  <- depmixS4::depmix(current ~ 1, data=X, nstates=7,
                                     family=gaussian())
            set.seed(42) # To make the random starting values repeatable.
            fit3 <- depmixS4::fit(mdl,emcontrol=em.control(maxit=1000))
        }
    }

## End(Not run)
```

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