Package: biogram (via r-universe)

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Type Package

Title N-Gram Analysis of Biological Sequences

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Description Tools for extraction and analysis of various n-grams (k-mers) derived from biological sequences (proteins or nucleic acids). Contains QuiPT (quick permutation test) for fast feature-filtering of the n-gram data.

License GPL-3

URL https://github.com/michbur/biogram

BugReports https://github.com/michbur/biogram/issues

VignetteBuilder knitr

Depends R (>= 3.0.0), slam

Imports combinat, entropy, partitions

Suggests ggplot2, knitr, testthat

NeedsCompilation no

Encoding UTF-8

RoxygenNote 7.1.0

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`biogram-package` *biogram - analysis of biological sequences using n-grams*

Description

`biogram` package is a toolbox for the analysis of nucleic acid and protein sequences using n-grams. Possible applications include motif discovery, feature selection, clustering, and classification.

n-grams

n-grams (k-tuples) are sets of `n` characters derived from the input sequence(s). They may form continuous sub-sequences or be discontinuous. For example, from the sequence of nucleotides `AATA` one can extract the following continuous 2-grams (bigrams): `AA`, `AT` and `TA`. Moreover, there are two possible bigrams separated by a single space: `A_T` and `A_A`, and one bigram separated by two spaces: `A__A`.

Another important n-gram parameter is its position. Instead of just counting n-grams, one may want to count how many n-grams occur at a given position in multiple (e.g. related) sequences. For example, in the sequences `AATA` and `AACA` there is only one bigram at position 1: `AA`, but there are two bigrams at position two: `AT` and `AC`. The following notation is used for position-specific n-grams: `1_AA`, `2_AT`, `2_AC`.

In the `biogram` package, the `count_ngrams` function is used for counting and extracting n-grams. Using the `d` argument the user can specify the distance between elements of the n-grams. The `pos` argument can be used to enable position specificity.

n-gram data dimensionality

We note that n-grams suffer from the curse of dimensionality. For example, for a peptide of length 6 20^n n-grams and 6×20^n positioned n-grams are possible. Data sets of such an enormous size are hard to manage and analyze in R.

The `biogram` package deals with both of the abovementioned problems. It uses innate properties of the n-gram data which usually can be represented by sparse matrices. Data storage is done using functionalities from the `slam` package. To ease the selection of significant features, `biogram` provides the user with QuiPT, a very fast permutation test for binary data (see `test_features`).

Another way of reducing dimensionality is the aggregation of sequence residues into more general groups. For example, all positively-charged amino acids may be aggregated into one group. This action can be performed using the `degenerate` function.

Encoding of amino acids can easu sequence analysis, but multidimensional objects as the aggregations of amino acids are not easily comparable. We introduced the encoding distance, a measure defining the distance between encodings. It can be computed using the `calc_ed` function.

Author(s)

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Examples

```
# use data set from package
data(human_cleave)
# first nine columns represent subsequent nine amino acids from cleavage sites
# degenerate the sequence to reduce the dimensionality of the problem
# (use five groups instead of 20 amino acids)
deg_seqs <- degenerate(human_cleave[, 1L:9],
                       list(`a` = c(1, 6, 8, 10, 11, 18),
                            `b` = c(2, 13, 14, 16, 17),
                            `c` = c(5, 19, 20),
                            `d` = c(7, 9, 12, 15),
                            'e' = c(3, 4)))
# EXAMPLE 1 - extract significant trigrams
# extract trigrams
trigrams <- count_ngrams(deg_seqs, 3, letters[1L:5], pos = TRUE)
# select features that differ between the two target groups using QuiPT
test1 <- test_features(human_cleave[, "tar"], trigrams)
# see a summary of the results
summary(test1)
# aggregate features in groups based on their p-value
gr <- cut(test1)
# get position map of the most significant n-grams
position_ngrams(gr[[1]])
# transform the most significant n-grams to more readable form
decode_ngrams(gr[[1]])

# EXAMPLE 2 - search for specific n-grams
# the n-grams of the interest are a_a (a-gap-a) and e_e (e-gap-e) on the
# 3rd and 4th position
# firstly code n-grams in biogram notation and add position information
```

```
coded <- code_ngrams(c("a_a", "c_c"))
# add position information
coded <- c(paste0("3_", coded), paste0("4_", coded))
# count only the features of the interest
bigrams <- count_specified(deg_seqs, coded)
# test which of the features of the interest is significant
test2 <- test_features(human_cleave[, "tar"], bigrams)
cut(test2)
```

---

aaprop *Normalized amino acids properties*

Description

Normalized (0-1) 554 amino acid properties as retreived from AAIndex database (release 9.1) enriched with contactivity of amino acids.

Format

A data frames with 20 columns and 600 rows.

Details

Following properties are included (AAIndex key: description of the property)

ANDN920101 alpha-CH chemical shifts (Andersen et al., 1992)

ARGP820101 Hydrophobicity index (Argos et al., 1982)

ARGP820102 Signal sequence helical potential (Argos et al., 1982)

ARGP820103 Membrane-buried preference parameters (Argos et al., 1982)

BEGF750101 Conformational parameter of inner helix (Beghin-Dirkx, 1975)

BEGF750102 Conformational parameter of beta-structure (Beghin-Dirkx, 1975)

BEGF750103 Conformational parameter of beta-turn (Beghin-Dirkx, 1975)

BHAR880101 Average flexibility indices (Bhaskaran-Ponnuswamy, 1988)

BIGC670101 Residue volume (Bigelow, 1967)

BIOV880101 Information value for accessibility; average fraction 35% (Biou et al., 1988)

BIOV880102 Information value for accessibility; average fraction 23% (Biou et al., 1988)

BROC820101 Retention coefficient in TFA (Browne et al., 1982)

BROC820102 Retention coefficient in HFBA (Browne et al., 1982)

BULH740101 Transfer free energy to surface (Bull-Breese, 1974)

BULH740102 Apparent partial specific volume (Bull-Breese, 1974)

BUNA790101 alpha-NH chemical shifts (Bundi-Wuthrich, 1979)

BUNA790102 alpha-CH chemical shifts (Bundi-Wuthrich, 1979)

BUNA790103 Spin-spin coupling constants 3JHalpha-NH (Bundi-Wuthrich, 1979)

BURA740101 Normalized frequency of alpha-helix (Burgess et al., 1974)

BURA740102 Normalized frequency of extended structure (Burgess et al., 1974)

CHAM810101 Steric parameter (Charton, 1981)

CHAM820101 Polarizability parameter (Charton-Charton, 1982)

CHAM820102 Free energy of solution in water, kcal/mole (Charton-Charton, 1982)

CHAM830101 The Chou-Fasman parameter of the coil conformation (Charton-Charton, 1983)

CHAM830102 A parameter defined from the residuals obtained from the best correlation of the Chou-Fasman parameter of beta-sheet (Charton-Charton, 1983)

CHAM830103 The number of atoms in the side chain labelled 1+1 (Charton-Charton, 1983)

CHAM830104 The number of atoms in the side chain labelled 2+1 (Charton-Charton, 1983)

CHAM830105 The number of atoms in the side chain labelled 3+1 (Charton-Charton, 1983)

CHAM830106 The number of bonds in the longest chain (Charton-Charton, 1983)

CHAM830107 A parameter of charge transfer capability (Charton-Charton, 1983)

CHAM830108 A parameter of charge transfer donor capability (Charton-Charton, 1983)

CHOC750101 Average volume of buried residue (Chothia, 1975)

CHOC760101 Residue accessible surface area in tripeptide (Chothia, 1976)

CHOC760102 Residue accessible surface area in folded protein (Chothia, 1976)

CHOC760103 Proportion of residues 95% buried (Chothia, 1976)

CHOC760104 Proportion of residues 100% buried (Chothia, 1976)

CHOP780101 Normalized frequency of beta-turn (Chou-Fasman, 1978a)

CHOP780201 Normalized frequency of alpha-helix (Chou-Fasman, 1978b)

CHOP780202 Normalized frequency of beta-sheet (Chou-Fasman, 1978b)

CHOP780203 Normalized frequency of beta-turn (Chou-Fasman, 1978b)

CHOP780204 Normalized frequency of N-terminal helix (Chou-Fasman, 1978b)

CHOP780205 Normalized frequency of C-terminal helix (Chou-Fasman, 1978b)

CHOP780206 Normalized frequency of N-terminal non helical region (Chou-Fasman, 1978b)

CHOP780207 Normalized frequency of C-terminal non helical region (Chou-Fasman, 1978b)

CHOP780208 Normalized frequency of N-terminal beta-sheet (Chou-Fasman, 1978b)

CHOP780209 Normalized frequency of C-terminal beta-sheet (Chou-Fasman, 1978b)

CHOP780210 Normalized frequency of N-terminal non beta region (Chou-Fasman, 1978b)

CHOP780211 Normalized frequency of C-terminal non beta region (Chou-Fasman, 1978b)

CHOP780212 Frequency of the 1st residue in turn (Chou-Fasman, 1978b)

CHOP780213 Frequency of the 2nd residue in turn (Chou-Fasman, 1978b)

CHOP780214 Frequency of the 3rd residue in turn (Chou-Fasman, 1978b)

CHOP780215 Frequency of the 4th residue in turn (Chou-Fasman, 1978b)

CHOP780216 Normalized frequency of the 2nd and 3rd residues in turn (Chou-Fasman, 1978b)

CIDH920101 Normalized hydrophobicity scales for alpha-proteins (Cid et al., 1992)

CIDH920102 Normalized hydrophobicity scales for beta-proteins (Cid et al., 1992)

CIDH920103 Normalized hydrophobicity scales for alpha+beta-proteins (Cid et al., 1992)

CIDH920104 Normalized hydrophobicity scales for alpha/beta-proteins (Cid et al., 1992)

CIDH920105 Normalized average hydrophobicity scales (Cid et al., 1992)

COHE430101 Partial specific volume (Cohn-Edsall, 1943)

CRAJ730101 Normalized frequency of middle helix (Crawford et al., 1973)

CRAJ730102 Normalized frequency of beta-sheet (Crawford et al., 1973)

CRAJ730103 Normalized frequency of turn (Crawford et al., 1973)

DAWD720101 Size (Dawson, 1972)

DAYM780101 Amino acid composition (Dayhoff et al., 1978a)

DAYM780201 Relative mutability (Dayhoff et al., 1978b)

DESM900101 Membrane preference for cytochrome b: MPH89 (Degli Esposti et al., 1990)

DESM900102 Average membrane preference: AMP07 (Degli Esposti et al., 1990)

EISD840101 Consensus normalized hydrophobicity scale (Eisenberg, 1984)

EISD860101 Solvation free energy (Eisenberg-McLachlan, 1986)

EISD860102 Atom-based hydrophobic moment (Eisenberg-McLachlan, 1986)

EISD860103 Direction of hydrophobic moment (Eisenberg-McLachlan, 1986)

FASG760101 Molecular weight (Fasman, 1976)

FASG760102 Melting point (Fasman, 1976)

FASG760103 Optical rotation (Fasman, 1976)

FASG760104 pK-N (Fasman, 1976)

FASG760105 pK-C (Fasman, 1976)

FAUJ830101 Hydrophobic parameter pi (Fauchere-Pliska, 1983)

FAUJ880101 Graph shape index (Fauchere et al., 1988)

FAUJ880102 Smoothed upsilon steric parameter (Fauchere et al., 1988)

FAUJ880103 Normalized van der Waals volume (Fauchere et al., 1988)

FAUJ880104 STERIMOL length of the side chain (Fauchere et al., 1988)

FAUJ880105 STERIMOL minimum width of the side chain (Fauchere et al., 1988)

FAUJ880106 STERIMOL maximum width of the side chain (Fauchere et al., 1988)

FAUJ880107 N.m.r. chemical shift of alpha-carbon (Fauchere et al., 1988)

FAUJ880108 Localized electrical effect (Fauchere et al., 1988)

FAUJ880109 Number of hydrogen bond donors (Fauchere et al., 1988)

FAUJ880110 Number of full nonbonding orbitals (Fauchere et al., 1988)

FAUJ880111 Positive charge (Fauchere et al., 1988)

FAUJ880112 Negative charge (Fauchere et al., 1988)

FAUJ880113 pK-a(RCOOH) (Fauchere et al., 1988)

FINA770101 Helix-coil equilibrium constant (Finkelstein-Ptitsyn, 1977)

FINA910101 Helix initiation parameter at posision i-1 (Finkelstein et al., 1991)
FINA910102 Helix initiation parameter at posision i,i+1,i+2 (Finkelstein et al., 1991)
FINA910103 Helix termination parameter at posision j-2,j-1,j (Finkelstein et al., 1991)
FINA910104 Helix termination parameter at posision j+1 (Finkelstein et al., 1991)
GARJ730101 Partition coefficient (Garel et al., 1973)
GEIM800101 Alpha-helix indices (Geisow-Roberts, 1980)
GEIM800102 Alpha-helix indices for alpha-proteins (Geisow-Roberts, 1980)
GEIM800103 Alpha-helix indices for beta-proteins (Geisow-Roberts, 1980)
GEIM800104 Alpha-helix indices for alpha/beta-proteins (Geisow-Roberts, 1980)
GEIM800105 Beta-strand indices (Geisow-Roberts, 1980)
GEIM800106 Beta-strand indices for beta-proteins (Geisow-Roberts, 1980)
GEIM800107 Beta-strand indices for alpha/beta-proteins (Geisow-Roberts, 1980)
GEIM800108 Aperiodic indices (Geisow-Roberts, 1980)
GEIM800109 Aperiodic indices for alpha-proteins (Geisow-Roberts, 1980)
GEIM800110 Aperiodic indices for beta-proteins (Geisow-Roberts, 1980)
GEIM800111 Aperiodic indices for alpha/beta-proteins (Geisow-Roberts, 1980)
GOLD730101 Hydrophobicity factor (Goldsack-Chalifoux, 1973)
GOLD730102 Residue volume (Goldsack-Chalifoux, 1973)
GRAR740101 Composition (Grantham, 1974)
GRAR740102 Polarity (Grantham, 1974)
GRAR740103 Volume (Grantham, 1974)
GUYH850101 Partition energy (Guy, 1985)
HOPA770101 Hydration number (Hopfinger, 1971), Cited by Charton-Charton (1982)
HOPT810101 Hydrophilicity value (Hopp-Woods, 1981)
HUTJ700101 Heat capacity (Hutchens, 1970)
HUTJ700102 Absolute entropy (Hutchens, 1970)
HUTJ700103 Entropy of formation (Hutchens, 1970)
ISOY800101 Normalized relative frequency of alpha-helix (Isogai et al., 1980)
ISOY800102 Normalized relative frequency of extended structure (Isogai et al., 1980)
ISOY800103 Normalized relative frequency of bend (Isogai et al., 1980)
ISOY800104 Normalized relative frequency of bend R (Isogai et al., 1980)
ISOY800105 Normalized relative frequency of bend S (Isogai et al., 1980)
ISOY800106 Normalized relative frequency of helix end (Isogai et al., 1980)
ISOY800107 Normalized relative frequency of double bend (Isogai et al., 1980)
ISOY800108 Normalized relative frequency of coil (Isogai et al., 1980)
JANJ780101 Average accessible surface area (Janin et al., 1978)
JANJ780102 Percentage of buried residues (Janin et al., 1978)

JANJ780103 Percentage of exposed residues (Janin et al., 1978)
JANJ790101 Ratio of buried and accessible molar fractions (Janin, 1979)
JANJ790102 Transfer free energy (Janin, 1979)
JOND750101 Hydrophobicity (Jones, 1975)
JOND750102 pK (-COOH) (Jones, 1975)
JOND920101 Relative frequency of occurrence (Jones et al., 1992)
JOND920102 Relative mutability (Jones et al., 1992)
JUKT750101 Amino acid distribution (Jukes et al., 1975)
JUNJ780101 Sequence frequency (Jungck, 1978)
KANM800101 Average relative probability of helix (Kanehisa-Tsong, 1980)
KANM800102 Average relative probability of beta-sheet (Kanehisa-Tsong, 1980)
KANM800103 Average relative probability of inner helix (Kanehisa-Tsong, 1980)
KANM800104 Average relative probability of inner beta-sheet (Kanehisa-Tsong, 1980)
KARP850101 Flexibility parameter for no rigid neighbors (Karplus-Schulz, 1985)
KARP850102 Flexibility parameter for one rigid neighbor (Karplus-Schulz, 1985)
KARP850103 Flexibility parameter for two rigid neighbors (Karplus-Schulz, 1985)
KHAG800101 The Kerr-constant increments (Khanarian-Moore, 1980)
KLEP840101 Net charge (Klein et al., 1984)
KRIW710101 Side chain interaction parameter (Krigbaum-Rubin, 1971)
KRIW790101 Side chain interaction parameter (Krigbaum-Komoriya, 1979)
KRIW790102 Fraction of site occupied by water (Krigbaum-Komoriya, 1979)
KRIW790103 Side chain volume (Krigbaum-Komoriya, 1979)
KYTJ820101 Hydropathy index (Kyte-Doolittle, 1982)
LAWE840101 Transfer free energy, CHP/water (Lawson et al., 1984)
LEVM760101 Hydrophobic parameter (Levitt, 1976)
LEVM760102 Distance between C-alpha and centroid of side chain (Levitt, 1976)
LEVM760103 Side chain angle theta(AAR) (Levitt, 1976)
LEVM760104 Side chain torsion angle phi(AAAR) (Levitt, 1976)
LEVM760105 Radius of gyration of side chain (Levitt, 1976)
LEVM760106 van der Waals parameter R0 (Levitt, 1976)
LEVM760107 van der Waals parameter epsilon (Levitt, 1976)
LEVM780101 Normalized frequency of alpha-helix, with weights (Levitt, 1978)
LEVM780102 Normalized frequency of beta-sheet, with weights (Levitt, 1978)
LEVM780103 Normalized frequency of reverse turn, with weights (Levitt, 1978)
LEVM780104 Normalized frequency of alpha-helix, unweighted (Levitt, 1978)
LEVM780105 Normalized frequency of beta-sheet, unweighted (Levitt, 1978)
LEVM780106 Normalized frequency of reverse turn, unweighted (Levitt, 1978)

LEWP710101 Frequency of occurrence in beta-bends (Lewis et al., 1971)
LIFS790101 Conformational preference for all beta-strands (Lifson-Sander, 1979)
LIFS790102 Conformational preference for parallel beta-strands (Lifson-Sander, 1979)
LIFS790103 Conformational preference for antiparallel beta-strands (Lifson-Sander, 1979)
MANP780101 Average surrounding hydrophobicity (Manavalan-Ponnuswamy, 1978)
MAXF760101 Normalized frequency of alpha-helix (Maxfield-Scheraga, 1976)
MAXF760102 Normalized frequency of extended structure (Maxfield-Scheraga, 1976)
MAXF760103 Normalized frequency of zeta R (Maxfield-Scheraga, 1976)
MAXF760104 Normalized frequency of left-handed alpha-helix (Maxfield-Scheraga, 1976)
MAXF760105 Normalized frequency of zeta L (Maxfield-Scheraga, 1976)
MAXF760106 Normalized frequency of alpha region (Maxfield-Scheraga, 1976)
MCMT640101 Refractivity (McMeekin et al., 1964), Cited by Jones (1975)
MEEJ800101 Retention coefficient in HPLC, pH7.4 (Meek, 1980)
MEEJ800102 Retention coefficient in HPLC, pH2.1 (Meek, 1980)
MEEJ810101 Retention coefficient in NaClO4 (Meek-Rossetti, 1981)
MEEJ810102 Retention coefficient in NaH2PO4 (Meek-Rossetti, 1981)
MEIH800101 Average reduced distance for C-alpha (Meirovitch et al., 1980)
MEIH800102 Average reduced distance for side chain (Meirovitch et al., 1980)
MEIH800103 Average side chain orientation angle (Meirovitch et al., 1980)
MIYS850101 Effective partition energy (Miyazawa-Jernigan, 1985)
NAGK730101 Normalized frequency of alpha-helix (Nagano, 1973)
NAGK730102 Normalized frequency of bata-structure (Nagano, 1973)
NAGK730103 Normalized frequency of coil (Nagano, 1973)
NAKH900101 AA composition of total proteins (Nakashima et al., 1990)
NAKH900102 SD of AA composition of total proteins (Nakashima et al., 1990)
NAKH900103 AA composition of mt-proteins (Nakashima et al., 1990)
NAKH900104 Normalized composition of mt-proteins (Nakashima et al., 1990)
NAKH900105 AA composition of mt-proteins from animal (Nakashima et al., 1990)
NAKH900106 Normalized composition from animal (Nakashima et al., 1990)
NAKH900107 AA composition of mt-proteins from fungi and plant (Nakashima et al., 1990)
NAKH900108 Normalized composition from fungi and plant (Nakashima et al., 1990)
NAKH900109 AA composition of membrane proteins (Nakashima et al., 1990)
NAKH900110 Normalized composition of membrane proteins (Nakashima et al., 1990)
NAKH900111 Transmembrane regions of non-mt-proteins (Nakashima et al., 1990)
NAKH900112 Transmembrane regions of mt-proteins (Nakashima et al., 1990)
NAKH900113 Ratio of average and computed composition (Nakashima et al., 1990)
NAKH920101 AA composition of CYT of single-spanning proteins (Nakashima-Nishikawa, 1992)

NAKH920102 AA composition of CYT2 of single-spanning proteins (Nakashima-Nishikawa, 1992)
NAKH920103 AA composition of EXT of single-spanning proteins (Nakashima-Nishikawa, 1992)
NAKH920104 AA composition of EXT2 of single-spanning proteins (Nakashima-Nishikawa, 1992)
NAKH920105 AA composition of MEM of single-spanning proteins (Nakashima-Nishikawa, 1992)
NAKH920106 AA composition of CYT of multi-spanning proteins (Nakashima-Nishikawa, 1992)
NAKH920107 AA composition of EXT of multi-spanning proteins (Nakashima-Nishikawa, 1992)
NAKH920108 AA composition of MEM of multi-spanning proteins (Nakashima-Nishikawa, 1992)
NISK800101 8 A contact number (Nishikawa-Ooi, 1980)
NISK860101 14 A contact number (Nishikawa-Ooi, 1986)
NOZY710101 Transfer energy, organic solvent/water (Nozaki-Tanford, 1971)
OOBM770101 Average non-bonded energy per atom (Oobatake-Ooi, 1977)
OOBM770102 Short and medium range non-bonded energy per atom (Oobatake-Ooi, 1977)
OOBM770103 Long range non-bonded energy per atom (Oobatake-Ooi, 1977)
OOBM770104 Average non-bonded energy per residue (Oobatake-Ooi, 1977)
OOBM770105 Short and medium range non-bonded energy per residue (Oobatake-Ooi, 1977)
OOBM850101 Optimized beta-structure-coil equilibrium constant (Oobatake et al., 1985)
OOBM850102 Optimized propensity to form reverse turn (Oobatake et al., 1985)
OOBM850103 Optimized transfer energy parameter (Oobatake et al., 1985)
OOBM850104 Optimized average non-bonded energy per atom (Oobatake et al., 1985)
OOBM850105 Optimized side chain interaction parameter (Oobatake et al., 1985)
PALJ810101 Normalized frequency of alpha-helix from LG (Palau et al., 1981)
PALJ810102 Normalized frequency of alpha-helix from CF (Palau et al., 1981)
PALJ810103 Normalized frequency of beta-sheet from LG (Palau et al., 1981)
PALJ810104 Normalized frequency of beta-sheet from CF (Palau et al., 1981)
PALJ810105 Normalized frequency of turn from LG (Palau et al., 1981)
PALJ810106 Normalized frequency of turn from CF (Palau et al., 1981)
PALJ810107 Normalized frequency of alpha-helix in all-alpha class (Palau et al., 1981)
PALJ810108 Normalized frequency of alpha-helix in alpha+beta class (Palau et al., 1981)
PALJ810109 Normalized frequency of alpha-helix in alpha/beta class (Palau et al., 1981)
PALJ810110 Normalized frequency of beta-sheet in all-beta class (Palau et al., 1981)
PALJ810111 Normalized frequency of beta-sheet in alpha+beta class (Palau et al., 1981)
PALJ810112 Normalized frequency of beta-sheet in alpha/beta class (Palau et al., 1981)
PALJ810113 Normalized frequency of turn in all-alpha class (Palau et al., 1981)
PALJ810114 Normalized frequency of turn in all-beta class (Palau et al., 1981)
PALJ810115 Normalized frequency of turn in alpha+beta class (Palau et al., 1981)
PALJ810116 Normalized frequency of turn in alpha/beta class (Palau et al., 1981)
PARJ860101 HPLC parameter (Parker et al., 1986)

PLIV810101 Partition coefficient (Pliska et al., 1981)
PONP800101 Surrounding hydrophobicity in folded form (Ponnuswamy et al., 1980)
PONP800102 Average gain in surrounding hydrophobicity (Ponnuswamy et al., 1980)
PONP800103 Average gain ratio in surrounding hydrophobicity (Ponnuswamy et al., 1980)
PONP800104 Surrounding hydrophobicity in alpha-helix (Ponnuswamy et al., 1980)
PONP800105 Surrounding hydrophobicity in beta-sheet (Ponnuswamy et al., 1980)
PONP800106 Surrounding hydrophobicity in turn (Ponnuswamy et al., 1980)
PONP800107 Accessibility reduction ratio (Ponnuswamy et al., 1980)
PONP800108 Average number of surrounding residues (Ponnuswamy et al., 1980)
PRAM820101 Intercept in regression analysis (Prabhakaran-Ponnuswamy, 1982)
PRAM820102 Slope in regression analysis x 1.0E1 (Prabhakaran-Ponnuswamy, 1982)
PRAM820103 Correlation coefficient in regression analysis (Prabhakaran-Ponnuswamy, 1982)
PRAM900101 Hydrophobicity (Prabhakaran, 1990)
PRAM900102 Relative frequency in alpha-helix (Prabhakaran, 1990)
PRAM900103 Relative frequency in beta-sheet (Prabhakaran, 1990)
PRAM900104 Relative frequency in reverse-turn (Prabhakaran, 1990)
PTIO830101 Helix-coil equilibrium constant (Ptitsyn-Finkelstein, 1983)
PTIO830102 Beta-coil equilibrium constant (Ptitsyn-Finkelstein, 1983)
QIAN880101 Weights for alpha-helix at the window position of -6 (Qian-Sejnowski, 1988)
QIAN880102 Weights for alpha-helix at the window position of -5 (Qian-Sejnowski, 1988)
QIAN880103 Weights for alpha-helix at the window position of -4 (Qian-Sejnowski, 1988)
QIAN880104 Weights for alpha-helix at the window position of -3 (Qian-Sejnowski, 1988)
QIAN880105 Weights for alpha-helix at the window position of -2 (Qian-Sejnowski, 1988)
QIAN880106 Weights for alpha-helix at the window position of -1 (Qian-Sejnowski, 1988)
QIAN880107 Weights for alpha-helix at the window position of 0 (Qian-Sejnowski, 1988)
QIAN880108 Weights for alpha-helix at the window position of 1 (Qian-Sejnowski, 1988)
QIAN880109 Weights for alpha-helix at the window position of 2 (Qian-Sejnowski, 1988)
QIAN880110 Weights for alpha-helix at the window position of 3 (Qian-Sejnowski, 1988)
QIAN880111 Weights for alpha-helix at the window position of 4 (Qian-Sejnowski, 1988)
QIAN880112 Weights for alpha-helix at the window position of 5 (Qian-Sejnowski, 1988)
QIAN880113 Weights for alpha-helix at the window position of 6 (Qian-Sejnowski, 1988)
QIAN880114 Weights for beta-sheet at the window position of -6 (Qian-Sejnowski, 1988)
QIAN880115 Weights for beta-sheet at the window position of -5 (Qian-Sejnowski, 1988)
QIAN880116 Weights for beta-sheet at the window position of -4 (Qian-Sejnowski, 1988)
QIAN880117 Weights for beta-sheet at the window position of -3 (Qian-Sejnowski, 1988)
QIAN880118 Weights for beta-sheet at the window position of -2 (Qian-Sejnowski, 1988)
QIAN880119 Weights for beta-sheet at the window position of -1 (Qian-Sejnowski, 1988)

QIAN880120 Weights for beta-sheet at the window position of 0 (Qian-Sejnowski, 1988)
QIAN880121 Weights for beta-sheet at the window position of 1 (Qian-Sejnowski, 1988)
QIAN880122 Weights for beta-sheet at the window position of 2 (Qian-Sejnowski, 1988)
QIAN880123 Weights for beta-sheet at the window position of 3 (Qian-Sejnowski, 1988)
QIAN880124 Weights for beta-sheet at the window position of 4 (Qian-Sejnowski, 1988)
QIAN880125 Weights for beta-sheet at the window position of 5 (Qian-Sejnowski, 1988)
QIAN880126 Weights for beta-sheet at the window position of 6 (Qian-Sejnowski, 1988)
QIAN880127 Weights for coil at the window position of -6 (Qian-Sejnowski, 1988)
QIAN880128 Weights for coil at the window position of -5 (Qian-Sejnowski, 1988)
QIAN880129 Weights for coil at the window position of -4 (Qian-Sejnowski, 1988)
QIAN880130 Weights for coil at the window position of -3 (Qian-Sejnowski, 1988)
QIAN880131 Weights for coil at the window position of -2 (Qian-Sejnowski, 1988)
QIAN880132 Weights for coil at the window position of -1 (Qian-Sejnowski, 1988)
QIAN880133 Weights for coil at the window position of 0 (Qian-Sejnowski, 1988)
QIAN880134 Weights for coil at the window position of 1 (Qian-Sejnowski, 1988)
QIAN880135 Weights for coil at the window position of 2 (Qian-Sejnowski, 1988)
QIAN880136 Weights for coil at the window position of 3 (Qian-Sejnowski, 1988)
QIAN880137 Weights for coil at the window position of 4 (Qian-Sejnowski, 1988)
QIAN880138 Weights for coil at the window position of 5 (Qian-Sejnowski, 1988)
QIAN880139 Weights for coil at the window position of 6 (Qian-Sejnowski, 1988)
RACS770101 Average reduced distance for C-alpha (Rackovsky-Scheraga, 1977)
RACS770102 Average reduced distance for side chain (Rackovsky-Scheraga, 1977)
RACS770103 Side chain orientational preference (Rackovsky-Scheraga, 1977)
RACS820101 Average relative fractional occurrence in A0(i) (Rackovsky-Scheraga, 1982)
RACS820102 Average relative fractional occurrence in AR(i) (Rackovsky-Scheraga, 1982)
RACS820103 Average relative fractional occurrence in AL(i) (Rackovsky-Scheraga, 1982)
RACS820104 Average relative fractional occurrence in EL(i) (Rackovsky-Scheraga, 1982)
RACS820105 Average relative fractional occurrence in E0(i) (Rackovsky-Scheraga, 1982)
RACS820106 Average relative fractional occurrence in ER(i) (Rackovsky-Scheraga, 1982)
RACS820107 Average relative fractional occurrence in A0(i-1) (Rackovsky-Scheraga, 1982)
RACS820108 Average relative fractional occurrence in AR(i-1) (Rackovsky-Scheraga, 1982)
RACS820109 Average relative fractional occurrence in AL(i-1) (Rackovsky-Scheraga, 1982)
RACS820110 Average relative fractional occurrence in EL(i-1) (Rackovsky-Scheraga, 1982)
RACS820111 Average relative fractional occurrence in E0(i-1) (Rackovsky-Scheraga, 1982)
RACS820112 Average relative fractional occurrence in ER(i-1) (Rackovsky-Scheraga, 1982)
RACS820113 Value of theta(i) (Rackovsky-Scheraga, 1982)
RACS820114 Value of theta(i-1) (Rackovsky-Scheraga, 1982)

RADA880101 Transfer free energy from chx to wat (Radzicka-Wolfenden, 1988)
RADA880102 Transfer free energy from oct to wat (Radzicka-Wolfenden, 1988)
RADA880103 Transfer free energy from vap to chx (Radzicka-Wolfenden, 1988)
RADA880104 Transfer free energy from chx to oct (Radzicka-Wolfenden, 1988)
RADA880105 Transfer free energy from vap to oct (Radzicka-Wolfenden, 1988)
RADA880106 Accessible surface area (Radzicka-Wolfenden, 1988)
RADA880107 Energy transfer from out to in(95%buried) (Radzicka-Wolfenden, 1988)
RADA880108 Mean polarity (Radzicka-Wolfenden, 1988)
RICJ880101 Relative preference value at N" (Richardson-Richardson, 1988)
RICJ880102 Relative preference value at N' (Richardson-Richardson, 1988)
RICJ880103 Relative preference value at N-cap (Richardson-Richardson, 1988)
RICJ880104 Relative preference value at N1 (Richardson-Richardson, 1988)
RICJ880105 Relative preference value at N2 (Richardson-Richardson, 1988)
RICJ880106 Relative preference value at N3 (Richardson-Richardson, 1988)
RICJ880107 Relative preference value at N4 (Richardson-Richardson, 1988)
RICJ880108 Relative preference value at N5 (Richardson-Richardson, 1988)
RICJ880109 Relative preference value at Mid (Richardson-Richardson, 1988)
RICJ880110 Relative preference value at C5 (Richardson-Richardson, 1988)
RICJ880111 Relative preference value at C4 (Richardson-Richardson, 1988)
RICJ880112 Relative preference value at C3 (Richardson-Richardson, 1988)
RICJ880113 Relative preference value at C2 (Richardson-Richardson, 1988)
RICJ880114 Relative preference value at C1 (Richardson-Richardson, 1988)
RICJ880115 Relative preference value at C-cap (Richardson-Richardson, 1988)
RICJ880116 Relative preference value at C' (Richardson-Richardson, 1988)
RICJ880117 Relative preference value at C" (Richardson-Richardson, 1988)
ROBB760101 Information measure for alpha-helix (Robson-Suzuki, 1976)
ROBB760102 Information measure for N-terminal helix (Robson-Suzuki, 1976)
ROBB760103 Information measure for middle helix (Robson-Suzuki, 1976)
ROBB760104 Information measure for C-terminal helix (Robson-Suzuki, 1976)
ROBB760105 Information measure for extended (Robson-Suzuki, 1976)
ROBB760106 Information measure for pleated-sheet (Robson-Suzuki, 1976)
ROBB760107 Information measure for extended without H-bond (Robson-Suzuki, 1976)
ROBB760108 Information measure for turn (Robson-Suzuki, 1976)
ROBB760109 Information measure for N-terminal turn (Robson-Suzuki, 1976)
ROBB760110 Information measure for middle turn (Robson-Suzuki, 1976)
ROBB760111 Information measure for C-terminal turn (Robson-Suzuki, 1976)
ROBB760112 Information measure for coil (Robson-Suzuki, 1976)

ROBB760113 Information measure for loop (Robson-Suzuki, 1976)
ROBB790101 Hydration free energy (Robson-Osguthorpe, 1979)
ROSG850101 Mean area buried on transfer (Rose et al., 1985)
ROSG850102 Mean fractional area loss (Rose et al., 1985)
ROSM880101 Side chain hydropathy, uncorrected for solvation (Roseman, 1988)
ROSM880102 Side chain hydropathy, corrected for solvation (Roseman, 1988)
ROSM880103 Loss of Side chain hydropathy by helix formation (Roseman, 1988)
SIMZ760101 Transfer free energy (Simon, 1976), Cited by Charton-Charton (1982)
SNEP660101 Principal component I (Sneath, 1966)
SNEP660102 Principal component II (Sneath, 1966)
SNEP660103 Principal component III (Sneath, 1966)
SNEP660104 Principal component IV (Sneath, 1966)
SUEM840101 Zimm-Bragg parameter s at 20 C (Sueki et al., 1984)
SUEM840102 Zimm-Bragg parameter sigma x 1.0E4 (Sueki et al., 1984)
SWER830101 Optimal matching hydrophobicity (Sweet-Eisenberg, 1983)
TANS770101 Normalized frequency of alpha-helix (Tanaka-Scheraga, 1977)
TANS770102 Normalized frequency of isolated helix (Tanaka-Scheraga, 1977)
TANS770103 Normalized frequency of extended structure (Tanaka-Scheraga, 1977)
TANS770104 Normalized frequency of chain reversal R (Tanaka-Scheraga, 1977)
TANS770105 Normalized frequency of chain reversal S (Tanaka-Scheraga, 1977)
TANS770106 Normalized frequency of chain reversal D (Tanaka-Scheraga, 1977)
TANS770107 Normalized frequency of left-handed helix (Tanaka-Scheraga, 1977)
TANS770108 Normalized frequency of zeta R (Tanaka-Scheraga, 1977)
TANS770109 Normalized frequency of coil (Tanaka-Scheraga, 1977)
TANS770110 Normalized frequency of chain reversal (Tanaka-Scheraga, 1977)
VASM830101 Relative population of conformational state A (Vasquez et al., 1983)
VASM830102 Relative population of conformational state C (Vasquez et al., 1983)
VASM830103 Relative population of conformational state E (Vasquez et al., 1983)
VELV850101 Electron-ion interaction potential (Veljkovic et al., 1985)
VENT840101 Bitterness (Venanzi, 1984)
VHEG790101 Transfer free energy to lipophilic phase (von Heijne-Blomberg, 1979)
WARP780101 Average interactions per side chain atom (Warme-Morgan, 1978)
WEBA780101 RF value in high salt chromatography (Weber-Lacey, 1978)
WERD780101 Propensity to be buried inside (Wertz-Scheraga, 1978)
WERD780102 Free energy change of epsilon(i) to epsilon(ex) (Wertz-Scheraga, 1978)
WERD780103 Free energy change of alpha(Ri) to alpha(Rh) (Wertz-Scheraga, 1978)
WERD780104 Free energy change of epsilon(i) to alpha(Rh) (Wertz-Scheraga, 1978)

WOEC730101 Polar requirement (Woese, 1973)

WOLR810101 Hydration potential (Wolfenden et al., 1981)

WOLS870101 Principal property value z1 (Wold et al., 1987)

WOLS870102 Principal property value z2 (Wold et al., 1987)

WOLS870103 Principal property value z3 (Wold et al., 1987)

YUTK870101 Unfolding Gibbs energy in water, pH7.0 (Yutani et al., 1987)

YUTK870102 Unfolding Gibbs energy in water, pH9.0 (Yutani et al., 1987)

YUTK870103 Activation Gibbs energy of unfolding, pH7.0 (Yutani et al., 1987)

YUTK870104 Activation Gibbs energy of unfolding, pH9.0 (Yutani et al., 1987)

ZASB820101 Dependence of partition coefficient on ionic strength (Zaslavsky et al., 1982)

ZIMJ680101 Hydrophobicity (Zimmerman et al., 1968)

ZIMJ680102 Bulkiness (Zimmerman et al., 1968)

ZIMJ680103 Polarity (Zimmerman et al., 1968)

ZIMJ680104 Isoelectric point (Zimmerman et al., 1968)

ZIMJ680105 RF rank (Zimmerman et al., 1968)

AURR980101 Normalized positional residue frequency at helix termini N4'(Aurora-Rose, 1998)

AURR980102 Normalized positional residue frequency at helix termini N"' (Aurora-Rose, 1998)

AURR980103 Normalized positional residue frequency at helix termini N" (Aurora-Rose, 1998)

AURR980104 Normalized positional residue frequency at helix termini N'(Aurora-Rose, 1998)

AURR980105 Normalized positional residue frequency at helix termini Nc (Aurora-Rose, 1998)

AURR980106 Normalized positional residue frequency at helix termini N1 (Aurora-Rose, 1998)

AURR980107 Normalized positional residue frequency at helix termini N2 (Aurora-Rose, 1998)

AURR980108 Normalized positional residue frequency at helix termini N3 (Aurora-Rose, 1998)

AURR980109 Normalized positional residue frequency at helix termini N4 (Aurora-Rose, 1998)

AURR980110 Normalized positional residue frequency at helix termini N5 (Aurora-Rose, 1998)

AURR980111 Normalized positional residue frequency at helix termini C5 (Aurora-Rose, 1998)

AURR980112 Normalized positional residue frequency at helix termini C4 (Aurora-Rose, 1998)

AURR980113 Normalized positional residue frequency at helix termini C3 (Aurora-Rose, 1998)

AURR980114 Normalized positional residue frequency at helix termini C2 (Aurora-Rose, 1998)

AURR980115 Normalized positional residue frequency at helix termini C1 (Aurora-Rose, 1998)

AURR980116 Normalized positional residue frequency at helix termini Cc (Aurora-Rose, 1998)

AURR980117 Normalized positional residue frequency at helix termini C' (Aurora-Rose, 1998)

AURR980118 Normalized positional residue frequency at helix termini C" (Aurora-Rose, 1998)

AURR980119 Normalized positional residue frequency at helix termini C"' (Aurora-Rose, 1998)

AURR980120 Normalized positional residue frequency at helix termini C4' (Aurora-Rose, 1998)

ONEK900101 Delta G values for the peptides extrapolated to 0 M urea (O'Neil-DeGrado, 1990)

ONEK900102 Helix formation parameters (delta delta G) (O'Neil-DeGrado, 1990)

VINM940101 Normalized flexibility parameters (B-values), average (Vihinen et al., 1994)

VINM940102 Normalized flexibility parameters (B-values) for each residue surrounded by none rigid neighbours (Vihinen et al., 1994)

VINM940103 Normalized flexibility parameters (B-values) for each residue surrounded by one rigid neighbours (Vihinen et al., 1994)

VINM940104 Normalized flexibility parameters (B-values) for each residue surrounded by two rigid neighbours (Vihinen et al., 1994)

MUNV940101 Free energy in alpha-helical conformation (Munoz-Serrano, 1994)

MUNV940102 Free energy in alpha-helical region (Munoz-Serrano, 1994)

MUNV940103 Free energy in beta-strand conformation (Munoz-Serrano, 1994)

MUNV940104 Free energy in beta-strand region (Munoz-Serrano, 1994)

MUNV940105 Free energy in beta-strand region (Munoz-Serrano, 1994)

WIMW960101 Free energies of transfer of AcWl-X-LL peptides from bilayer interface to water (Wimley-White, 1996)

KIMC930101 Thermodynamic beta sheet propensity (Kim-Berg, 1993)

MONM990101 Turn propensity scale for transmembrane helices (Monne et al., 1999)

BLAM930101 Alpha helix propensity of position 44 in T4 lysozyme (Blaber et al., 1993)

PARS000101 p-Values of mesophilic proteins based on the distributions of B values (Parthasarathy-Murthy, 2000)

PARS000102 p-Values of thermophilic proteins based on the distributions of B values (Parthasarathy-Murthy, 2000)

KUMS000101 Distribution of amino acid residues in the 18 non-redundant families of thermophilic proteins (Kumar et al., 2000)

KUMS000102 Distribution of amino acid residues in the 18 non-redundant families of mesophilic proteins (Kumar et al., 2000)

KUMS000103 Distribution of amino acid residues in the alpha-helices in thermophilic proteins (Kumar et al., 2000)

KUMS000104 Distribution of amino acid residues in the alpha-helices in mesophilic proteins (Kumar et al., 2000)

TAKK010101 Side-chain contribution to protein stability (kJ/mol) (Takano-Yutani, 2001)

FODM020101 Propensity of amino acids within pi-helices (Fodje-Al-Karadaghi, 2002)

NADH010101 Hydropathy scale based on self-information values in the two-state model (5% accessibility) (Naderi-Manesh et al., 2001)

NADH010102 Hydropathy scale based on self-information values in the two-state model (9% accessibility) (Naderi-Manesh et al., 2001)

NADH010103 Hydropathy scale based on self-information values in the two-state model (16% accessibility) (Naderi-Manesh et al., 2001)

NADH010104 Hydropathy scale based on self-information values in the two-state model (20% accessibility) (Naderi-Manesh et al., 2001)

NADH010105 Hydropathy scale based on self-information values in the two-state model (25% accessibility) (Naderi-Manesh et al., 2001)

NADH010106 Hydropathy scale based on self-information values in the two-state model (36% accessibility) (Naderi-Manesh et al., 2001)

NADH010107 Hydropathy scale based on self-information values in the two-state model (50% accessibility) (Naderi-Manesh et al., 2001)

MONM990201 Averaged turn propensities in a transmembrane helix (Monne et al., 1999)

KOEP990101 Alpha-helix propensity derived from designed sequences (Koehl-Levitt, 1999)

KOEP990102 Beta-sheet propensity derived from designed sequences (Koehl-Levitt, 1999)

CEDJ970101 Composition of amino acids in extracellular proteins (percent) (Cedano et al., 1997)

CEDJ970102 Composition of amino acids in anchored proteins (percent) (Cedano et al., 1997)

CEDJ970103 Composition of amino acids in membrane proteins (percent) (Cedano et al., 1997)

CEDJ970104 Composition of amino acids in intracellular proteins (percent) (Cedano et al., 1997)

CEDJ970105 Composition of amino acids in nuclear proteins (percent) (Cedano et al., 1997)

FUKS010101 Surface composition of amino acids in intracellular proteins of thermophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010102 Surface composition of amino acids in intracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010103 Surface composition of amino acids in extracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010104 Surface composition of amino acids in nuclear proteins (percent) (Fukuchi-Nishikawa, 2001)

FUKS010105 Interior composition of amino acids in intracellular proteins of thermophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010106 Interior composition of amino acids in intracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010107 Interior composition of amino acids in extracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010108 Interior composition of amino acids in nuclear proteins (percent) (Fukuchi-Nishikawa, 2001)

FUKS010109 Entire chain composition of amino acids in intracellular proteins of thermophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010110 Entire chain composition of amino acids in intracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010111 Entire chain composition of amino acids in extracellular proteins of mesophiles (percent) (Fukuchi-Nishikawa, 2001)

FUKS010112 Entire chain compositino of amino acids in nuclear proteins (percent) (Fukuchi-Nishikawa, 2001)

AVBF000101 Screening coefficients gamma, local (Avbelj, 2000)

AVBF000102 Screening coefficients gamma, non-local (Avbelj, 2000)

AVBF000103 Slopes tripeptide, FDPB VFF neutral (Avbelj, 2000)

AVBF000104 Slopes tripeptides, LD VFF neutral (Avbelj, 2000)

AVBF000105 Slopes tripeptide, FDPB VFF noside (Avbelj, 2000)

AVBF000106 Slopes tripeptide FDPB VFF all (Avbelj, 2000)

AVBF000107 Slopes tripeptide FDPB PARSE neutral (Avbelj, 2000)

AVBF000108 Slopes dekapeptide, FDPB VFF neutral (Avbelj, 2000)

AVBF000109 Slopes proteins, FDPB VFF neutral (Avbelj, 2000)

YANJ020101 Side-chain conformation by gaussian evolutionary method (Yang et al., 2002)

MITS020101 Amphiphilicity index (Mitaku et al., 2002)

TSAJ990101 Volumes including the crystallographic waters using the ProtOr (Tsai et al., 1999)

TSAJ990102 Volumes not including the crystallographic waters using the ProtOr (Tsai et al., 1999)

COSI940101 Electron-ion interaction potential values (Cosic, 1994)

PONP930101 Hydrophobicity scales (Ponnuswamy, 1993)

WILM950101 Hydrophobicity coefficient in RP-HPLC, C18 with 0.1%TFA/MeCN/H2O (Wilce et al. 1995)

WILM950102 Hydrophobicity coefficient in RP-HPLC, C8 with 0.1%TFA/MeCN/H2O (Wilce et al. 1995)

WILM950103 Hydrophobicity coefficient in RP-HPLC, C4 with 0.1%TFA/MeCN/H2O (Wilce et al. 1995)

WILM950104 Hydrophobicity coefficient in RP-HPLC, C18 with 0.1%TFA/2-PrOH/MeCN/H2O (Wilce et al. 1995)

KUHL950101 Hydrophilicity scale (Kuhn et al., 1995)

GUOD860101 Retention coefficient at pH 2 (Guo et al., 1986)

JURD980101 Modified Kyte-Doolittle hydrophobicity scale (Juretic et al., 1998)

BASU050101 Interactivity scale obtained from the contact matrix (Bastolla et al., 2005)

BASU050102 Interactivity scale obtained by maximizing the mean of correlation coefficient over single-domain globular proteins (Bastolla et al., 2005)

BASU050103 Interactivity scale obtained by maximizing the mean of correlation coefficient over pairs of sequences sharing the TIM barrel fold (Bastolla et al., 2005)

SUYM030101 Linker propensity index (Suyama-Ohara, 2003)

PUNT030101 Knowledge-based membrane-propensity scale from 1D_Helix in MPtopo databases (Punta-Maritan, 2003)

PUNT030102 Knowledge-based membrane-propensity scale from 3D_Helix in MPtopo databases (Punta-Maritan, 2003)

GEOR030101 Linker propensity from all dataset (George-Heringa, 2003)

GEOR030102 Linker propensity from 1-linker dataset (George-Heringa, 2003)

GEOR030103 Linker propensity from 2-linker dataset (George-Heringa, 2003)

GEOR030104 Linker propensity from 3-linker dataset (George-Heringa, 2003)

GEOR030105 Linker propensity from small dataset (linker length is less than six residues) (George-Heringa, 2003)

GEOR030106 Linker propensity from medium dataset (linker length is between six and 14 residues) (George-Heringa, 2003)

GEOR030107 Linker propensity from long dataset (linker length is greater than 14 residues) (George-Heringa, 2003)

GEOR030108 Linker propensity from helical (annotated by DSSP) dataset (George-Heringa, 2003)

GEOR030109 Linker propensity from non-helical (annotated by DSSP) dataset (George-Heringa, 2003)

ZHOH040101 The stability scale from the knowledge-based atom-atom potential (Zhou-Zhou, 2004)

ZHOH040102 The relative stability scale extracted from mutation experiments (Zhou-Zhou, 2004)

ZHOH040103 Buriability (Zhou-Zhou, 2004)

BAEK050101 Linker index (Bae et al., 2005)

HARY940101 Mean volumes of residues buried in protein interiors (Harpaz et al., 1994)

PONJ960101 Average volumes of residues (Pontius et al., 1996)

DIGM050101 Hydrostatic pressure asymmetry index, PAI (Di Giulio, 2005)

WOLR790101 Hydrophobicity index (Wolfenden et al., 1979)

OLSK800101 Average internal preferences (Olsen, 1980)

KIDA850101 Hydrophobicity-related index (Kidera et al., 1985)

GUYH850102 Apparent partition energies calculated from Wertz-Scheraga index (Guy, 1985)

GUYH850103 Apparent partition energies calculated from Robson-Osguthorpe index (Guy, 1985)

GUYH850104 Apparent partition energies calculated from Janin index (Guy, 1985)

GUYH850105 Apparent partition energies calculated from Chothia index (Guy, 1985)

ROSM880104 Hydropathies of amino acid side chains, neutral form (Roseman, 1988)

ROSM880105 Hydropathies of amino acid side chains, pi-values in pH 7.0 (Roseman, 1988)

JACR890101 Weights from the IFH scale (Jacobs-White, 1989)

COWR900101 Hydrophobicity index, 3.0 pH (Cowan-Whittaker, 1990)

BLAS910101 Scaled side chain hydrophobicity values (Black-Mould, 1991)

CASG920101 Hydrophobicity scale from native protein structures (Casari-Sippl, 1992)

CORJ870101 NNEIG index (Cornette et al., 1987)

CORJ870102 SWEIG index (Cornette et al., 1987)

CORJ870103 PRIFT index (Cornette et al., 1987)

CORJ870104 PRILS index (Cornette et al., 1987)

CORJ870105 ALTFT index (Cornette et al., 1987)

CORJ870106 ALTLS index (Cornette et al., 1987)

CORJ870107 TOTFT index (Cornette et al., 1987)

CORJ870108 TOTLS index (Cornette et al., 1987)

MIYS990101 Relative partition energies derived by the Bethe approximation (Miyazawa-Jernigan, 1999)

MIYS990102 Optimized relative partition energies - method A (Miyazawa-Jernigan, 1999)

MIYS990103 Optimized relative partition energies - method B (Miyazawa-Jernigan, 1999)

MIYS990104 Optimized relative partition energies - method C (Miyazawa-Jernigan, 1999)

MIYS990105 Optimized relative partition energies - method D (Miyazawa-Jernigan, 1999)

ENGD860101 Hydrophobicity index (Engelman et al., 1986)

FASG890101 Hydrophobicity index (Fasman, 1989)

K6.5 Values of Wc in proteins from class Beta, cutoff 6 A, separation 5 (Wozniak, 2014)

K8.5 Values of Wc in proteins from class Beta, cutoff 8 A, separation 5 (Wozniak, 2014)

K12.5 Values of Wc in proteins from class Beta, cutoff 12 A, separation 5 (Wozniak, 2014)

K6.15 Values of Wc in proteins from class Beta, cutoff 6 A, separation 15 (Wozniak, 2014)

K8.15 Values of Wc in proteins from class Beta, cutoff 8 A, separation 15 (Wozniak, 2014)

K12.15 Values of Wc in proteins from class Beta, cutoff 12 A, separation 15 (Wozniak, 2014)

Source

AAIndex database.

References

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Wozniak, P. and Kotulska M. (2014) Characteristics of protein residue-residue contacts and their application in contact prediction. 20(11):2497

Examples

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data(aaprop)
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`add_1grams` *Add 1-grams*

Description

Builds (n+1)-grams from n-grams.

Usage

```
add_1grams(ngram, u, seq_length)
```

Arguments

`ngram`	a single n-gram.
`u`	`integer`, `numeric` or `character` vector of all possible unigrams.
`seq_length`	length of an origin sequence.

Details

n-grams are built by pasting every possible unigram in the every possible free position. The total length of n-gram (n plus total distance between elements of the n-gram) is limited by the length of an origin sequence, because the n-gram cannot be longer than an origin sequence.

Value

vector of n-grams (where n is equal to the n of the input plus one).

See Also

Reverse function: gap_ngrams.

Examples

```
add_1grams("1_2.3.4_3.0", 1L:4, 8)

add_1grams("a.a_1", c("a", "b", "c"), 4)
```

---

as.data.frame.feature_test

Coerce feature_test object to a data frame

Description

Coerce results of test_features function to a data.frame.

Usage

```
## S3 method for class 'feature_test'
as.data.frame(
  x,
  row.names = NULL,
  optional = FALSE,
  stringsAsFactors = FALSE,
  ...
)
```

Arguments

x	object of class feature_test.
row.names	ignored.
optional	ignored.
stringsAsFactors	logical: should the character vector be converted to a factor?.
...	additional arguments to be passed to or from methods.

Value

a data frame with four columns: names of n-gram, p-values, occurrences in positive and negative sequences.

`binarize` *Binarize*

Description

Binarizes a matrix.

Usage

```
binarize(x)
```

Arguments

`x`	`matrix` or `simple_triplet_matrix`.

Value

a `matrix` or `simple_triplet_matrix` (depending on the input).

`calc_criterion` *Calculate value of criterion*

Description

Computes a chosen statistical criterion for each feature versus target vector.

Usage

```
calc_criterion(target, features, criterion_function)
```

Arguments

`target`	`integer` vector with target information (e.g. class labels).
`features`	`integer` matrix of features with number of rows equal to the length of the target vector.
`criterion_function`	a function calculating criterion. For a full list, see `test_features`.

Details

The permutation test implemented in `biogram` uses several criterions to filter important features. Each can be used by `test_features` by specifying the `criterion` parameter.

Value

a `integer` vector of length equal to the number of features containing computed information gain values.

Note

Both `target` and `features` must be binary, i.e. contain only 0 and 1 values.

See Also

`test_features`.

Examples

```
tar <- sample(0L:1, 100, replace = TRUE)
feats <- matrix(sample(0L:1, 400, replace = TRUE), ncol = 4)

# Information Gain
calc_criterion(tar, feats, calc_ig)

# hi-squared-based measure
calc_criterion(tar, feats, calc_cs)

# Kullback-Leibler divergence
calc_criterion(tar, feats, calc_kl)
```

---

calc_cs *Calculate Chi-squared-based measure*

Description

Computes Chi-squared-based measure between features and target vector.

Usage

```
calc_cs(feature, target, len_target, pos_target)
```

Arguments

`feature`	feature vector.
`target`	target.
`len_target`	length of the target vector.
`pos_target`	number of positive cases in the target vector.

Value

A `numeric` vector of length 1 representing computed Chi-square values.

Note

Both `target` and `features` must be binary, i.e. contain only 0 and 1 values.

The function was designed to be as fast as possible subroutine of `calc_criterion` and might be cumbersome if directly called by a user.

See Also

`test_features`.

`chisq.test` - Pearson's chi-squared test for count data.

Examples

```
tar <- sample(0L:1, 100, replace = TRUE)
feat <- sample(0L:1, 100, replace = TRUE)
calc_cs(feat, tar, 100, sum(tar))
```

---

calc_ed *Calculate encoding distance*

Description

Computes the encoding distance between two encodings.

Usage

```
calc_ed(a, b, prop = NULL, measure)
```

Arguments

`a`	encoding (see `validate_encoding` for more information about the required structure of encoding).
`b`	encoding to which `a` should be compared. Must have equal number of groups or less than `a`. Both `a` and `b` must have the the same number of elements.
`prop`	`matrix` of physicochemical properties to normalize the encoding distance. Each column should represent properties of the single amino acid/nucleotide. If `NULL`, encoding distance is not normalized.
`measure`	`character` vector of length one specifying the measure. Currently avaible measures are `"pi"` (partition index) and `"si"` (similarity index). If the parameter `prop` is supplied, the encoding distance is normalized by the factor equal to the sum of distances for each group in `a` and the closest group in `b`. The position of a group is defined as the mean value of properties of amino acids or nucleotides belonging the group. See the package vignette for more details.

Value

an encoding distance.

See Also

calc_si: compute the similarity index of two encodings. encoding2df: converts an encoding to a data frame. validate_encoding: validate a structure of an encoding.

Examples

```
# calculate encoding distance between two encodings of amino acids
aa1 = list(`1` = c("g", "a", "p", "v", "m", "l", "i"),
           `2` = c("k", "h"),
           `3` = c("d", "e"),
           `4` = c("f", "r", "w", "y", "s", "t", "c", "n", "q"))

aa2 = list(`1` = c("g", "a", "p", "v", "m", "l", "q"),
           `2` = c("k", "h", "d", "e", "i"),
           `3` = c("f", "r", "w", "y", "s", "t", "c", "n"))
calc_ed(aa1, aa2, measure = "pi")

# the encoding distance between two identical encodings is 0
calc_ed(aa1, aa1, measure = "pi")
```

---

calc_ig *Calculate IG for single feature*

Description

Computes information gain of single feature and target vector.

Usage

```
calc_ig(feature, target, len_target, pos_target)
```

Arguments

feature	feature vector.
target	target.
len_target	length of the target vector.
pos_target	number of positive cases in the target vector.

Details

The information gain term is used here (improperly) as a synonym of mutual information. It is defined as:

$$IG(X;Y) = \sum_{y \in Y} \sum_{x \in X} p(x,y) \log \left(\frac{p(x,y)}{p(x)p(y)} \right)$$

In biogram package information gain is computed using following relationship: $IG = E(S) - E(S|F)$

Value

A numeric vector of length 1 representing information gain in nats.

Note

During calculations $0 \log 0 = 0$. For a justification see References.

The function was designed to be afast subroutine of calc_criterion and might be cumbersome if directly called by a user.

References

Cover TM, Thomas JA *Elements of Information Theory, 2nd Edition* Wiley, 2006.

Examples

```
tar <- sample(0L:1, 100, replace = TRUE)
feat <- sample(0L:1, 100, replace = TRUE)
calc_ig(feat, tar, 100, sum(tar))
```

---

calc_kl *Calculate KL divergence of features*

Description

Computes Kullback-Leibler divergence between features and target vector.

Usage

```
calc_kl(feature, target, len_target, pos_target)
```

Arguments

feature	feature vector.
target	target.
len_target	length of the target vector.
pos_target	number of positive cases in the target vector.

Value

A numeric vector of length 1 representing Kullback-Leibler divergence value.

Note

Both target and features must be binary, i.e. contain only 0 and 1 values.

The function was designed to be as fast as possible subroutine of calc_criterion and might be cumbersome if directly called by a user.

References

Kullback S, Leibler RA *On information and sufficiency*. Annals of Mathematical Statistics 22 (1):79-86, 1951.

See Also

`test_features`. Kullback-Leibler divergence is calculated using `KL.plugin`.

Examples

```
tar <- sample(0L:1, 100, replace = TRUE)
feat <- sample(0L:1, 100, replace = TRUE)
calc_kl(feat, tar, 100, sum(tar))
```

`calc_pi` *Calculate partition index*

Description

Computes the encoding distance between two encodings.

Usage

```
calc_pi(a, b)
```

Arguments

`a`	encoding (see `validate_encoding` for more information about the required structure of encoding).
`b`	encoding to which `a` should be compared. Must have equal number of groups or less than `a`. Both `a` and `b` must have the the same number of elements.

Details

The encoding distance between `a` and `b` is defined as the minimum number of amino acids that have to be moved between subgroups of encoding to make `a` identical to `b` (order of subgroups in the encoding and amino acids in a group is unimportant).

If the parameter `prop` is supplied, the encoding distance is normalized by the factor equal to the sum of distances for each group in `a` and the closest group in `b`. The position of a group is defined as the mean value of properties of amino acids or nucleotides belonging the group.

See the package vignette for more details.

Value

an encoding distance.

See Also

calc_si: compute the similarity index of two encodings. encoding2df: converts an encoding to a data frame. validate_encoding: validate a structure of an encoding.

Examples

```
# calculate encoding distance between two encodings of amino acids
aa1 = list(`1` = c("g", "a", "p", "v", "m", "l", "i"),
           `2` = c("k", "h"),
           `3` = c("d", "e"),
           `4` = c("f", "r", "w", "y", "s", "t", "c", "n", "q"))

aa2 = list(`1` = c("g", "a", "p", "v", "m", "l", "q"),
           `2` = c("k", "h", "d", "e", "i"),
           `3` = c("f", "r", "w", "y", "s", "t", "c", "n"))
calc_pi(aa1, aa2)

# the encoding distance between two identical encodings is 0
calc_pi(aa1, aa1)
```

---

calc_si *Compute similarity index*

Description

Computes similarity index between two encodings.

Usage

```
calc_si(a, b)
```

Arguments

a	encoding (see validate_encoding for more information about the required structure of encoding).
b	encoding to which a should be compared. Must have equal number of groups or less than a. Both a and b must have the the same number of elements.

Details

Briefly, the similarity index is a fraction of elements that have the same pairing in both encodings. Pairing is a binary variable, that has value 1 if two elements are in the same group and 0 if not. For more details, see references.

Value

the value of similarity index.

References

Stephenson, J.D., and Freeland, S.J. (2013). Unearthing the Root of Amino Acid Similarity. J Mol Evol 77, 159-169.

See Also

`calc_ed`: calculate the encoding distance between two encodings.

Examples

```
# example from Stephenson & Freeland, 2013 (Fig. 6)
enc1 <- list(`1` = "A",
             `2` = c("F", "E"),
             `3` = c("C", "D", "G"))

enc2 <- list(`1` = c("A", "G"),
             `2` = c("C", "D", "E", "F"))

enc3 <- list(`1` = c("D", "G"),
             `2` = c("E", "F"),
             `3` = c("A", "C"))

calc_si(enc1, enc2)
calc_si(enc2, enc3)
calc_si(enc1, enc3)
```

---

check_criterion *Check chosen criterion*

Description

Checks if the criterion is viable or matches it to the list of implemented criterions.

Usage

```
check_criterion(input_criterion, criterion_names = c("ig", "kl", "cs"))
```

Arguments

`input_criterion`
: `character` string, criterion from input.

`criterion_names`
: list of implemented criterions, always in lowercase.

Value

a list of three:

- criterion name,
- its function,
- nice name for outputs.

See Also

Calculate the value of criterion: `calc_criterion`.

`cluster_reg_exp` *Clustering of sequences based on regular expression*

Description

Clusters sequences hierarchically with regular expressions. At each step we minimize number of degrees of freedom for all regular expressions needed to describe the data

Usage

```
cluster_reg_exp(ngrams)
```

Arguments

`ngrams`	list of elements

Details

Regular expression is a list of the length equal to the length of the input sequences. Each element of the list represents a position in the sequence and contains amino acid, that are likely to occure on this position.

Value

List of four

- "regExps"regular expression in best clustering
- "seqClustering"clustering of sequences in best clustering
- "allRegExps"all regular expressions.
- "allIndices"all clusterings

Examples

```
data(human_cleave)
#cluster_reg_exp is computationally expensive

results <- cluster_reg_exp(human_cleave[1L:10, 1L:4])
```

code_ngrams *Code n-grams*

Description

Code human-friendly representation of n-grams into a biogram format.

Usage

```
code_ngrams(decoded_ngrams)
```

Arguments

decoded_ngrams	a character vector of decoded n-grams.

Value

a character vector of n-grams.

See Also

Inverse function: decode_ngrams.

Examples

```
code_ngrams(c("11_2", "1__12", "222"))
code_ngrams(c("aaa_b", "d__aa", "abd"))
```

construct_ngrams *Construct and filter n-grams*

Description

Builds and selects important n-grams stepwise.

Usage

```
construct_ngrams(
  target,
  seq,
  u,
  n_max,
  conf_level = 0.95,
  gap = TRUE,
  use_heuristics = TRUE
)
```

Arguments

target	integer vector with target information (e.g. class labels).
seq	a vector or matrix describing sequence(s).
u	integer, numeric or character vector of all possible unigrams.
n_max	size of constructed n-grams.
conf_level	confidence level.
gap	logical, if TRUE gaps are used. See Details.
use_heuristics	if FALSE then all n-grams are tested. This may slow down computations significantly

Details

construct_ngrams starts by extracting unigrams from the sequences, pasting them together in all combination and choosing from them significant features (with p-value below conf_level). The chosen n-grams are further extended to the specified by n_max size by pasting unigrams at both ends.

The gap parameter determines if construct_ngrams performs the feature selection on exact n-grams (gap equal to FALSE) or on all features in the Hamming distance 1 from the n-gram (gap equal to TRUE).

Value

a vector of n-grams.

See Also

Feature filtering method: test_features.

Examples

```
# to make the example faster, we run construct_ngrams() on the
# subset of data
deg_seqs <- degenerate(human_cleave[c(1L:100, 801L:900), 1L:9],
list(`1` = c(1, 6, 8, 10, 11, 18),
     `2` = c(2, 13, 14, 16, 17),
     `3` = c(5, 19, 20),
     `4` = c(7, 9, 12, 15),
     '5' = c(3, 4)))
bigrams <- construct_ngrams(human_cleave[c(1L:100, 801L:900), "tar"], deg_seqs, 1L:5, 2)
```

count_multigrams *Detect and count multiple n-grams in sequences*

Description

A convinient wrapper around count_ngrams for counting multiple values of n and d.

Usage

```
count_multigrams(
  ns,
  ds = rep(0, length(ns)),
  seq,
  u,
  pos = FALSE,
  scale = FALSE,
  threshold = 0
)
```

Arguments

ns	numeric vector of n-grams' sizes. See Details.
ds	list of distances between elements of n-grams. Each element of the list is a vector used as distance for the respective n-gram size given by the ns parameter.
seq	a vector or matrix describing sequence(s).
u	integer, numeric or character vector of all possible unigrams.
pos	logical, if TRUE position-specific n_grams are counted.
scale	logical, if TRUE output data is normalized. May be applied only to the counts of n-grams without position information. See Details.
threshold	integer, if not equal to 0, data is binarized into two groups (larger or equal to threshold vs. smaller than threshold).

Details

ns vector and ds vector must have equal length. Elements of ds vector are used as equivalents of d parameter for respective values of ns. For example, if ns is c(4, 4, 4), the ds must be a list of length 3. Each element of the ds list must have length 3 or 1, as appropriate for a d parameter in count_ngrams function.

Value

An integer matrix with named columns. The naming conventions are the same as in count_ngrams.

Examples

```
seqs <- matrix(sample(1L:4, 600, replace = TRUE), ncol = 50)
count_multigrams(c(3, 1), list(c(1, 0), 0), seqs, 1L:4, pos = TRUE)
# if ds parameter is not present, n-grams are calculated for distance 0
count_multigrams(c(3, 1), seq = seqs, u = 1L:4)

# calculate three times n-gram with the same length, but different distances between
# elements
count_multigrams(c(4, 4, 4), list(c(2, 0, 1), c(2, 1, 0), c(0, 1, 2)),
                 seqs, 1L:4, pos = TRUE)
```

---

count_ngrams *Count n-grams in sequences*

Description

Counts all n-grams or position-specific n-grams present in the input sequence(s).

Usage

```
count_ngrams(seq, n, u, d = 0, pos = FALSE, scale = FALSE, threshold = 0)
```

Arguments

seq	a vector or matrix describing sequence(s).
n	integer size of n-gram.
u	integer, numeric or character vector of all possible unigrams.
d	integer vector of distances between elements of n-gram (0 means consecutive elements). See Details.
pos	logical, if TRUE position-specific n_grams are counted.
scale	logical, if TRUE output data is normalized. May be applied only to the counts of n-grams without position information. See Details.
threshold	integer, if not equal to 0, data is binarized into two groups (larger or equal to threshold vs. smaller than threshold).

Details

A distance vector should be always n - 1 in length. For example when n = 3, d = c(1,2) means A_A__A. For n = 4, d = c(2,0,1) means A__AA_A. If vector d has length 1, it is recycled to length n - 1.

n-gram names follow a specific convention and have three parts for position-specific n-grams and two parts otherwise. The parts are separated by _. The . symbol is used to separate elements within a part. The general naming scheme is POSITION_NGRAM_DISTANCE. The optional POSITION part of the name indicates the actual position of the n-gram in the sequence(s) and will be present only if pos = TRUE. This part is always a single integer. The NGRAM part of the name is a sequence of

elements in the n-gram. For example, `4.2.2` indicates the n-gram 422 (e.g. TCC). The `DISTANCE` part of the name is a vector of distance(s). For example, `0.0` indicates zero distances (continuous n-grams), while `1.2` represents distances for the n-gram A_A__A.

Examples of n-gram names:

- 46_4.4.4_0.1 : trigram 44_4 on position 46
- 12_2.1_2 : bigram 2__1 on position 12
- 8_1.1.1_0.0 : continuous trigram 111 on position 8
- 1.1.1_0.0 : continuous trigram 111 without position information

Value

a `simple_triplet_matrix` where columns represent n-grams and rows sequences. See `Details` for specifics of the naming convention.

Note

By default, the counted n-gram data is stored in a memory-saving format. To convert an object to a 'classical' matrix use the `as.matrix` function. See examples for further information.

See Also

Create vector of possible n-grams: `create_ngrams`.

Extract n-grams from sequence(s): `seq2ngrams`.

Get indices of n-grams: `get_ngrams_ind`.

Count n-grams for multiple values of n: `count_multigrams`.

Count only specified n-grams: `count_specified`.

Examples

```
# count trigrams without position information for nucleotides
count_ngrams(sample(1L:4, 50, replace = TRUE), 3, 1L:4, pos = FALSE)
# count position-specific trigrams from multiple nucleotide sequences
seqs <- matrix(sample(1L:4, 600, replace = TRUE), ncol = 50)
ngrams <- count_ngrams(seqs, 3, 1L:4, pos = TRUE)
# output results of the n-gram counting to screen
as.matrix(ngrams)
```

count_specified *Count specified n-grams*

Description

Counts specified n-grams in the input sequence(s).

Usage

```
count_specified(seq, ngrams)
```

Arguments

seq	vector or matrix describing sequence(s).
ngrams	vector of n-grams.

Details

count_specified counts only selected n-grams declared by user in the ngrams parameter. Declared n-grams must be written using the biogram notation.

Value

A simple_triplet_matrix where columns represent n-grams and rows sequences.

See Also

Count all possible n-grams: count_ngrams.

Examples

```
seqs <- matrix(c(1, 2, 2, 1, 2, 1, 2, 1, 1, 2, 3, 4, 1, 2, 2, 4), nrow = 2)
count_specified(seqs, ngrams = c("1.1.1_0.0", "2.2.2_0.0", "1.1.2_0.0"))

seqs <- matrix(sample(1L:5, 200, replace = TRUE), nrow = 20)
count_specified(seqs, ngrams = c("2_4.2_0", "2_1.4_0", "3_1.3_0",
                                 "2_4.2_1", "2_1.4_1", "3_1.3_1",
                                 "2_4.2_2", "2_1.4_2", "3_1.3_2"))
```

`count_total` *Count total number of n-grams*

Description

Computes total number of n-grams that can be extracted from sequences.

Usage

```
count_total(seq, n, d)
```

Arguments

`seq`	a vector or matrix describing sequence(s).
`n`	`integer` size of n-gram.
`d`	`integer` vector of distances between elements of n-gram (0 means consecutive elements). See Details.

Details

The maximum number of possible n-grams is limited by their length and the distance between elements of the n-gram.

Value

An `integer` rperesenting the total number of n-grams.

Note

A format of `d` vector is discussed in Details of `count_ngrams`. The maximum

Examples

```
seqs <- matrix(sample(1L:4, 600, replace = TRUE), ncol = 50)
# make several sequences shorter by replacing them partially with NA
seqs[8L:11, 46L:50] <- NA
seqs[1L, 31L:50] <- NA
count_total(seqs, 3, c(1, 0))
```

`create_encoding` *Create encoding*

Description

Reduces an alphabet using physicochemical properties.

Usage

```
create_encoding(prop, len)
```

Arguments

`prop`	`matrix` of properties with number of column equal to the length of the alphabet. Column must be named after elements of the alphabet. Each row represents a different physicochemical property.
`len`	length of the resulting encoding. Must be larger than zero and smaller than number of elements in the alphabet.

Details

The encoding is a list of groups to which elements of an alphabet should be reduced. All elements of the alphabet (all amino acids or all nucleotides) should appear in the encoding.

Value

An encoding.

See Also

`calc_ed`: calculate the encoding distance between two encodings. `encoding2df`: converts an encoding to a data frame. `validate_encoding`: validate a structure of an encoding.

Examples

```
enc1 = list(`1` = c("a", "t"),
            `2` = c("g", "c"))
encoding2df(enc1)
```

create_feature_target *Create feature according to given contingency matrix*

Description

Creates a matrix of features and target based on the values from contingency matrix.

Usage

```
create_feature_target(n11, n01, n10, n00)
```

Arguments

n11	number of elements for which both target and feature equal 1.
n01	number of elements for which target and feature equal 1,0 respectively.
n10	number of elements for which target and feature equal 0,1 respectively.
n00	number of elements for which both target and feature equal 0.

Value

a matrix of 2 columns and n11+n10+n01+n00 rows. Columns represent target and feature vectors, respectively.

Examples

```
# equivalent of
#         target
# feature 10 375
#        15 600
target_feature <- create_feature_target(10, 375, 15, 600)
```

create_ngrams *Get all possible n-Grams*

Description

Creates the vector of all possible n_grams (for given n).

Usage

```
create_ngrams(n, u, possible_grams = NULL)
```

Arguments

n	integer size of n-gram.
u	integer, numeric or character vector of all possible unigrams.
possible_grams	number of possible n-grams. If not NULL n-grams do not contain information about position

Details

See Details section of count_ngrams for more information about n-grams naming convention. The possible information about distance must be added by hand (see examples).

Value

a character vector. Elements of n-gram are separated by dot.

Note

Input data must be a matrix or data frame of numeric elements.

Examples

```
# bigrams for standard aminoacids
create_ngrams(2, 1L:20)
# bigrams for standard aminoacids with positions, 10 amino acid long sequence, so
# only 9 bigrams can be located in sequence
create_ngrams(2, 1L:20, 9)
# bigrams for DNA with positions, 10 nucleotide long sequence, distance 1, so only
# 8 bigrams in sequence
# paste0 adds information about distance at the end of n-gram
paste0(create_ngrams(2, 1L:4, 8), "_0")
```

---

criterion_distribution

criterion_distribution class

Description

A result of distr_crit function.

Details

An object of class criterion_distribution is a numeric matrix.

Data

1st column: possible values of criterion.

2nd column: probability density function.

3rd column: cumulative distribution function.

Attributes

plot_data A matrix with values of the criterion and their probabilities.

nice_name 'Nice' name of the criterion.

---

cut.feature_test *Categorize tested features*

Description

Categorizes results of `test_features` function into groups based on their significance.

Usage

```
## S3 method for class 'feature_test'
cut(x, split = "significances", breaks = c(0, 1e-04, 0.01, 0.05, 1), ...)
```

Arguments

`x`	an object of class `feature_test`.
`split`	attribute along which output should be categorized. Possible values are `"significances"`, `"positives"` and `"negatives"`. See `Value`.
`breaks`	a vector of significances of frequencies along which n-grams are aggregated. See description of `cut` function and `Details`.
`...`	further parameters accepted by the `cut` function.

Value

the value of function depends on the `split` parameter. The function returns a named list of length equal to the length of `significances` (when `split` equals `"significances"`) or `frequencies` (when `split` equals `"positives"` or `"negatives"`) minus one. Each elements of the list contains names of the n-grams belonging to the given significance or frequency group.

---

decode_ngrams *Decode n-grams*

Description

Transforms a vector of n-grams into a human-friendly form.

Usage

```
decode_ngrams(ngrams)
```

Arguments

ngrams	a character vector of n-grams.

Value

a character vector of length equal to the number of n-grams.

Note

Decoded n-grams lose the position information.

See Also

Validate n-gram structure: is_ngram.

Inverse function: code_ngrams.

Examples

```
decode_ngrams(c("2_1.1.2_0.1", "3_1.1.2_2.0", "3_2.2.2_0.0"))
```

---

degenerate *Degenerate protein sequence*

Description

'Degenerates' amino acid or nucleic sequence by aggregating elements to bigger groups.

Usage

```
degenerate(seq, element_groups)
```

Arguments

seq	character vector or matrix representing single sequence.
element_groups	encoding of elements: list of groups to which elements of sequence should be aggregated. Must have unique names.

Value

A character vector or matrix (if input is a matrix) containing aggregated elements.

Note

Characters not present in the element_groups will be converted to NA with a warning.

See Also

l2n to easily convert information stored in biological sequences from letters to numbers. calc_ed to calculate distance between encodings.

Examples

```
sample_seq <- c(1, 3, 1, 3, 4, 4, 3, 1, 2)
table(sample_seq)

# aggregate sequence to purins and pyrimidines
deg_seq <- degenerate(sample_seq, list(w = c(1, 4), s = c(2, 3)))
table(deg_seq)
```

---

degenerate_ngrams *Degenerate n-grams*

Description

'Degenerates' n-grams by aggregating amino acid or nucleotide elements into bigger groups.

Usage

```
degenerate_ngrams(x, element_groups, binarize = FALSE)
```

Arguments

x	object containing n-grams.
element_groups	encoding of elements: list of groups to which elements of n-grams should be aggregated. Must have unique names.
binarize	logical indicating if n-grams should be binarized

Value

A character vector or matrix (if input is a matrix) containing degenerated n-grams.

distr_crit *Compute criterion distribution*

Description

Computes criterion distribution under null hypothesis for all contingency tables possible for a feature and a target.

Usage

```
distr_crit(target, feature, criterion = "ig", iter_limit = 200)
```

Arguments

target	{0,1}-valued target vector. See Details.
feature	{0,1}-valued feature vector. See Details.
criterion	criterion used for calculations of distribution. See calc_criterion for the list of avaible criteria.
iter_limit	limit the number of calculated contingence matrices. If NULL, computes all possible contingence matrices.

Details

both target and feature vectors may contain only 0 and 1.

Value

An object of class criterion_distribution.

See Also

calc_criterion.

Examples

```
target_feature <- create_feature_target(10, 375, 15, 600)
distr_crit(target = target_feature[,1], feature = target_feature[,2])
```

encoding2df *Convert encoding to data frame*

Description

Converts an encoding to a data frame.

Usage

```
encoding2df(x, sort = FALSE)
```

Arguments

x	encoding.
sort	if TRUE rows are sorted according to elements.

Details

The encoding is a list of groups to which elements of an alphabet should be reduced. All elements of the alphabet (all amino acids or all nucleotides) should appear in the encoding.

Value

data frame with two columns. First column represents an index of a group in the supplied encoding and the second column contains all elements of the encoding.

See Also

calc_ed: calculate the encoding distance between two encodings. encoding2df: converts an encoding to a data frame. validate_encoding: validate a structure of an encoding.

Examples

```
create_encoding(aaprop[1L:5, ], 5)
```

fast_crosstable *2d cross-tabulation*

Description

Quickly cross-tabulates two binary vectors.

Usage

```
fast_crosstable(target, len_target, pos_target, feature)
```

Arguments

target	target.
len_target	length of the target vector.
pos_target	number of positive cases in the target vector.
feature	feature vector.

Details

Input looks odd, but the function was build to be fast subroutine of calc_ig, which works on many features but only one target.

Value

a vector of length four:

1. target +, feature+
2. target +, feature-
3. target -, feature+
4. target -, feature-

Note

Binary vector means a numeric vector with 0 or 1.

Examples

```
tar <- sample(0L:1, 100, replace = TRUE)
feat <- sample(0L:1, 100, replace = TRUE)
fast_crosstable(tar, length(tar), sum(tar),  feat)
```

---

feature_test *feature_test class*

Description

A result of test_features function.

Details

An object of the feature_test class is a numeric vector of p-values. Additional attributes characterizes futher the details of test which returned these p-values.

Attributes

criterion the criterion used in permutation test.

adjust the name of p-value adjusting method.

times the number of permutations. If QuiPT was chosen NA.

occ frequency of features splitted in subset based on the value of target.

See Also

Methods:

- as.data.frame.feature_test
- cut.feature_test
- print.feature_test
- summary.feature_test

---

full2simple *Convert encoding from full to simple format*

Description

Converts an encoding from the full format to the simple format.

Usage

```
full2simple(x)
```

Arguments

x	encoding.

Examples

```
aa1 = list(`1` = c("g", "a", "p", "v", "m", "l", "i"),
           `2` = c("k", "h"),
           `3` = c("d", "e"),
           `4` = c("f", "r", "w", "y", "s", "t", "c", "n", "q"))
full2simple(aa1)
```

gap_ngrams *Gap n-grams*

Description

Introduces gaps in the n-grams.

Usage

```
gap_ngrams(ngrams)
```

Arguments

ngrams	a vector of positioned n-grams (as created by count_ngrams).

Details

A single element of the input n-gram at a time will be replaced by a gap. For example, introducing gaps in n-gram 2_1.1.2_0.1 will results in three n-grams: 3_1.2_1 (where the 2_1_0 unigram was replaced by a gap), 2_1.2_2 and 2_1.1_0.

Value

A character vector of (n-1)-grams with introduced gaps.

See Also

Reverse function: add_1grams.

Examples

```
gap_ngrams(c("2_1.1.2_0.1", "3_1.1.2_0.0", "3_2.2.2_0.0"))
gap_ngrams(c("1.1.2_0.1", "1.1.2_0.0", "2.2.2_0.0"))
```

generate_sequence *Generate sequence*

Description

Generate a sequences using an alphabet of unigrams and set of rules.

Usage

```
generate_sequence(alphabet, regions)
```

Arguments

alphabet	the unigram alphabet. Columns are equivalent to unigrams and rows to particular properties.
regions	a list of rules describing regions.

---

generate_single_region

Generate single region

Description

Generate a region using an alphabet of unigrams and considering provided set of rules.

Usage

```
generate_single_region(alphabet, reg_len, prop_ranges, exactness)
```

Arguments

alphabet	the unigram alphabet. Columns are equivalent to unigrams and rows to particular properties.
reg_len	the number of unigrams inside the region.
prop_ranges	required intervals of properties of unigrams in the region. See Details.
exactness	a numeric value between 0 and 1 defining how stricly unigrams are kept within prop_ranges. If 1, only unigrams within prop_ranges are inside the region. if 0.9, there is 10 unigrams that are not in the prop_ranges will be inside the region.

Examples

```
props1 <- list(P1 = c(0, 0.5),
               P2 = c(0.2, 0.4),
               P3 = c(0.5, 1),
               P4 = c(0, 0))

props2 <- list(P1 = c(0.5, 1),
               P2 = c(0.4, 1),
               P3 = c(0, 0.5),
               P4 = c(1, 1))


alph <- generate_unigrams(c(replicate(8, props1, simplify = FALSE),
                            replicate(12, props2, simplify = FALSE)),
                          unigram_names = letters[1L:20])

rules1 <- list(P1 = c(0.5, 1),
               P2 = c(0.4, 1),
```

```
                P3 = c(0, 0.5),
                P4 = c(1, 1))

generate_single_region(alph, 10, rules1, 0.9)
```

`generate_single_unigram` *Generate single unigram*

Description

Assign randomly generated properties to a single unigram.

Usage

```
generate_single_unigram(unigram_ranges)
```

Arguments

`unigram_ranges`	list of ranges containing respective properties. If named, names are preserved.

See Also

`generate_single_unigram` is a helper function for `generate_unigrams`.

Examples

```
generate_single_unigram(list(P1 = c(0, 0.5),
                             P2 = c(0.2, 0.4),
                             P3 = c(0.5, 1),
                             P4 = c(0, 0)))
```

`generate_unigrams` *Generate unigrams*

Description

Generates an alphabet of unigrams based on given list of properties.

Usage

```
generate_unigrams(unigram_list, unigram_names = NULL, prop_names = NULL)
```

Arguments

unigram_list	a list of unigrams' parameters. See Details.
unigram_names	names of unigrams. If not NULL, will overwrite any existing unigram names.
prop_names	names of properties. If not NULL, will overwrite any existing names.

Details

Unigram parameters are represented as a list of intervals, where each interval corresponds to a different property. The function generate unigrams randomly choosing values of properties from given intervals using uniform distribution. All lists of ranges should have the same length, which equils to describing each unigram using the same properties.

Examples

```
props1 <- list(P1 = c(0, 0.5),
               P2 = c(0.2, 0.4),
               P3 = c(0.5, 1),
               P4 = c(0, 0))

props2 <- list(P1 = c(0.5, 1),
               P2 = c(0.4, 1),
               P3 = c(0, 0.5),
               P4 = c(1, 1))


alph <- generate_unigrams(c(replicate(8, props1, simplify = FALSE),
                            replicate(12, props2, simplify = FALSE)),
                            unigram_names = letters[1L:20])
```

---

get_ngrams_ind *Get indices of n-grams*

Description

Computes list of n-gram elements positions in sequence.

Usage

```
get_ngrams_ind(len_seq, n, d)
```

Arguments

len_seq	integer value describing sequence's length.
n	integer size of n-gram.
d	integer vector of distances between elements of n-gram (0 means consecutive elements). See Details.

Details

A format of d vector is discussed in Details of count_ngrams.

Value

A list with number of elements equal to n. Every element is a vector containing locations of given n-gram letter. For example, first element of list contain indices of first letter of all n-grams. The attribute d of output contains distances between letter used to compute locations (see Details).

Examples

```
# positions trigrams in sequence of length 10
get_ngrams_ind(10, 9, 0)
```

---

human_cleave *Human signal peptides cleavage sites*

Description

A set of 648 cleavage sites and 648 parts of mature proteins shortly after cleavage sites derived from human proteome.

Format

A data frame with 1296 observations on the following 10 variables. Columns from P1 to P9 describes positions in an extracted peptide. tar is a target vector. It has value 1 if a peptide is a cleavage site and 0 if not.

Details

Each peptide in the data set is nine amino acid residues long. In case of cleavage sites, the clevage is located between fifth and sixth peptide. The non-cleavage sites are parts of mature proteins starting five positions after cleavage site.

Note

Amino acid residues were recoded as integers.

Source

UniProt

Examples

```
data(human_cleave)
table(human_cleave[, 1])
```

is_ngram *Validate n-gram*

Description

Checks if the character string may be used as an n-gram and its notation follows specific convention of biogram package.

Usage

```
is_ngram(x)
```

Arguments

x	character string representing single n-gram.

Value

TRUE if n-gram's notation is correct, FALSE if not.

Examples

```
print(is_ngram("1_1.1.1_0.0"))
print(is_ngram("not_ngram"))
```

l2n *Convert letters to numbers*

Description

Converts biological sequence from letter to number notation.

Usage

```
l2n(seq, seq_type)
```

Arguments

seq	character vector or matrix representing single sequence.
seq_type	the type of sequence. Can be rna, dna or prot.

Value

a numeric vector or matrix containing converted elements.

See Also

l2n is a wrapper around degenerate.

Inverse function: n2l.

Examples

```
sample_seq <- c("a", "d", "d", "g", "a", "g", "n", "a", "l")
l2n(sample_seq, "prot")
```

---

list2matrix *Convert list of sequences to matrix*

Description

Converts list of sequences to matrix.

Usage

```
list2matrix(seq_list)
```

Arguments

seq_list	list of sequences (e.g. as returned by the read.fasta function).

Value

A matrix with the number of rows equal to the number of sequences and the number of columns equal to the length of the longest sequence.

Note

Since matrix must have specified number of columns, ends of shorter sequences are completed with NAs.

Examples

```
list2matrix(list(s1 = c("c", "g", "g", "t"),
                 s2 = c("g", "t", "c", "t", "t", "g"),
                 s3 = c("a", "a", "t")))
```

n2l *Convert numbers to letters*

Description

Converts biological sequence from number to letter notation.

Usage

```
n2l(seq, seq_type)
```

Arguments

seq	integer vector or matrix representing single sequence.
seq_type	the type of sequence. Can be rna, dna or prot.

Value

a character vector or matrix containing converted elements.

See Also

n2l is a wrapper around degenerate.

Inverse function: l2n.

Examples

```
sample_seq <- c(1, 3, 3, 6, 1, 6, 12, 1, 10)
n2l(sample_seq, "prot")
```

ngrams2df *n-grams to data frame*

Description

Tranforms a vector of n-grams into a data frame.

Usage

```
ngrams2df(ngrams)
```

Arguments

ngrams	a character vector of n-grams.

Value

a data.frame with 2 (in case of n-grams without known position) or three columns (n-grams with position information).

See Also

Decode n-grams: decode_ngrams.

Examples

```
ngrams2df(c("2_1.1.2_0.0", "3_1.1.2_0.0", "3_2.2.2_0.0", "2_1.1_0"))
```

---

plot.criterion_distribution

Plot criterion distribution

Description

Plots results of distr_crit function.

Usage

```
## S3 method for class 'criterion_distribution'
plot(x, ...)
```

Arguments

x	object of class criterion_distribution.
...	further arguments passed to plot.

Value

nothing.

Examples

```
target_feature <- create_feature_target(10, 375, 15, 600)
example_result <- distr_crit(target = target_feature[,1],
                             feature = target_feature[,2])
plot(example_result)

# a ggplot2 plot
library(ggplot2)
ggplot_distr <- function(x) {
b <- data.frame(cbind(x=as.numeric(rownames(attr(x, "plot_data"))),
                      attr(x, "plot_data")))
d1 <- cbind(b[,c(1,2)], attr(x, "nice_name"))
d2 <- cbind(b[,c(1,3)], "Probability")
```

```
colnames(d1) <- c("x", "y", "panel")
colnames(d2) <- c("x", "y", "panel")
d <- rbind(d1, d2)
p <- ggplot(data = d, mapping = aes(x = x, y = y)) +
  facet_grid(panel~., scale="free") +
  geom_freqpoly(data= d2, aes(color=y), stat = "identity") +
  scale_fill_brewer(palette = "Set1") +
  geom_point(data=d1, aes(size=y), stat = "identity") +
  guides(color = "none") +
  guides(size = "none") +
  xlab("Number of cases with feature=1 and target=1") + ylab("")
p
}
ggplot_distr(example_result)
```

`position_ngrams` *Position n-grams*

Description

Tranforms a vector of positioned n-grams into a list of positions filled with n-grams that start on them.

Usage

```
position_ngrams(ngrams, df = FALSE, unigrams_output = TRUE)
```

Arguments

`ngrams`	a vector of positioned n-grams (as created by `count_ngrams`).
`df`	logical, if `TRUE` returns a data frame, if `FALSE` returns a list.
`unigrams_output`	logical, if `TRUE` extracts unigrams from the data and returns information about their position.

Value

if `df` is `FALSE`, returns a list of length equal to the number of unique n-gram starts present in n-grams. Each element of the list contains n-grams that start on this position. If `df` is `FALSE`, returns a data frame where first column contains n-grams and the second column represent their start positions.

See Also

Transform n-gram name to human-friendly form: `decode_ngrams`.

Validate n-gram structure: `is_ngram`.

Examples

```
# position data in the list format
position_ngrams(c("2_1.1.2_0.1", "3_1.1.2_0.0", "3_2.2.2_0.0"))
# position data in the data frame format
position_ngrams(c("2_1.1.2_0.1", "3_1.1.2_0.0", "3_2.2.2_0.0"), df = TRUE)
```

---

print.feature_test *Print tested features*

Description

Prints results of test_features function.

Usage

```
## S3 method for class 'feature_test'
print(x, ...)
```

Arguments

x	object of class feature_test.
...	further arguments passed to print.default.

Value

nothing.

---

read_fasta *Read FASTA files*

Description

A lightweight tool to read nucleic or amino-acid sequences from a file in FASTA format.

Usage

```
read_fasta(file)
```

Arguments

file	the name of the file which the data are to be read from.

Value

a list of sequences.

See Also

read.fasta: heavier function for processing FASTA files.

Examples

```
## Not run:
  read_fasta("https://www.uniprot.org/uniprot/P28307.fasta")

## End(Not run)
```

---

regenerate *Regenerate n-grams*

Description

'Regenerates' amino acid or nucleic sequence written in a simplified alphabet by converting groups to regular expression.

Usage

```
regenerate(x, element_groups)
```

Arguments

x	character string representing single n-gram.
element_groups	encoding of elements: list of groups to which elements of sequence should be aggregated. Must have unique names.

Value

A character string representing a POSIX regular expression.

Note

Gaps (_) will be converted to any possible character from the alphabet (nucleotides or amino acids).

See Also

degenerate to easily convert information stored in biological sequences from letters to numbers.
calc_ed to calculate distance between simplified alphabets.

Examples

```
regenerate("ssw", list(w = c(1, 4), s = c(2, 3)))
```

regional_param *regional_param class*

Description

List of rules defining the region.

Details

An object of the `regional_param` class is a list consisting of all rules necessary to properly build a region.

Attributes

reg_len the number of unigrams inside the region. Might be 0

prop_ranges required intervals of properties of unigrams in the region

exactness a `numeric` value between 0 and 1 defining how stricly unigrams are kept within `prop_ranges`. If 1, only unigrams within `prop_ranges` are inside the region. if 0.9, there is 10 unigrams that are not in the `prop_ranges` will be inside the region.

See Also

`generate_sequence`

seq2ngrams *Extract n-grams from sequence*

Description

Extracts vector of n-grams present in sequence(s).

Usage

```
seq2ngrams(seq, n, u, d = 0, pos = FALSE)
```

Arguments

`seq`	a vector or matrix describing sequence(s).
`n`	`integer` size of n-gram.
`u`	`integer`, `numeric` or `character` vector of all possible unigrams.
`d`	`integer` vector of distances between elements of n-gram (0 means consecutive elements). See Details.
`pos`	`logical`, if `TRUE` position-specific n_grams are counted.

Details

A format of d vector is discussed in Details of count_ngrams.

Value

A character matrix of n-grams, where every row corresponds to a different sequence.

Examples

```
# trigrams from multiple sequences
seqs <- matrix(sample(1L:4, 600, replace = TRUE), ncol = 50)
seq2ngrams(seqs, 3, 1L:4)
```

---

simple2full *Convert encoding from simple to full format*

Description

Converts an encoding from the simple format to the full format.

Usage

```
simple2full(x)
```

Arguments

x	encoding (see Details).

Details

The encoding should be named. Each name should correspond to a different amino acid or nucleotide.

Examples

```
aa1 = structure(c("1", "4", "3", "3", "4", "1", "2", "1", "2", "1",
                  "1", "4", "1", "4", "4", "4", "4", "1", "4", "4"),
                .Names = c("a", "c", "d", "e", "f", "g", "h", "i",
                           "k", "l", "m", "n", "p", "q",
                           "r", "s", "t", "v", "w", "y"))
simple2full(aa1)
```

summary.feature_test *Summarize tested features*

Description

Summarizes results of `test_features` function.

Usage

```
## S3 method for class 'feature_test'
summary(object, conf_level = 0.95, ...)
```

Arguments

`object`	of class `feature_test`.
`conf_level`	confidence level. A feature with p-value equal to or smaller than the confidence is considered significant.
`...`	ignored

Value

nothing.

table_ngrams *Tabulate n-grams*

Description

Builds a contingency table of the n-gram counts versus their class labels.

Usage

```
table_ngrams(seq, ngrams, target)
```

Arguments

`seq`	vector or matrix describing sequence(s).
`ngrams`	vector of n-grams.
`target`	`integer` vector with target information (e.g. class labels). Must have at least two values.

Value

a data frame with the number of columns equal to the length of the `target` plus 1. The first column contains names of the n-grams. Further columns represents counts of n-grams for respective value of the `target`.

Examples

```
seqs_pos <- matrix(sample(c("a", "c", "g", "t"), 100, replace = TRUE,
            prob = c(0.2, 0.4, 0.35, 0.05)), ncol = 5)
seqs_neg <- matrix(sample(c("a", "c", "g", "t"), 100, replace = TRUE),
            ncol = 5)
tab <- table_ngrams(seq = rbind(seqs_pos, seqs_neg),
             ngrams = c("1_c.t_0", "1_g.g_0", "2_t.c_0", "2_g.g_0", "3_c.c_0", "3_g.c_0"),
                    target = c(rep(1, 20), rep(0, 20)))
# see the results
print(tab)
# easily plot the results using ggplot2
```

---

test_features *Permutation test for feature selection*

Description

Performs a feature selection on positioned n-gram data using a Fisher's permutation test.

Usage

```
test_features(
  target,
  features,
  criterion = "ig",
  adjust = "BH",
  threshold = 1,
  quick = TRUE,
  times = 1e+05
)
```

Arguments

target	integer vector with target information (e.g. class labels).
features	integer matrix of features with number of rows equal to the length of the target vector.
criterion	criterion used in permutation test. See Details for the list of possible criterions.
adjust	name of p-value adjustment method. See p.adjust for the list of possible values. If NULL, p-values are not adjusted.
threshold	integer. Features that occur less than threshold and more often than nrow(features)-threshold are discarded from the permutation test.
quick	logical, if TRUE Quick Permutation Test (QuiPT) is used. If FALSE, normal permutation test is performed.
times	number of times procedure should be repeated. Ignored if quick is TRUE.

Details

Since the procedure involves multiple testing, it is advisable to use one of the avaible p-value adjustment methods. Such methods can be used directly by specifying the `adjust` parameter.

Available criterions:

ig Information Gain: `calc_ig`.

kl Kullback-Leibler divergence: `calc_kl`.

cs Chi-squared-based measure: `calc_cs`.

Value

an object of class `feature_test`.

Note

Both `target` and `features` must be binary, i.e. contain only 0 and 1 values.

Features occuring too often and too rarely are considered not informative and may be removed using the threshold parameter.

References

Radivojac P, Obradovic Z, Dunker AK, Vucetic S, *Feature selection filters based on the permutation test* in Machine Learning: ECML 2004, 15th European Conference on Machine Learning, Springer, 2004.

See Also

`binarize` - binarizes input data.

`calc_criterion` - computes selected criterion.

`distr_crit` - distribution of criterion used in QuiPT.

`summary.feature_test` - summary of results.

`cut.feature_test` - aggregates test results in groups based on feature's p-value.

Examples

```
# significant feature
tar_feat1 <- create_feature_target(10, 390, 0, 600)
# significant feature
tar_feat2 <- create_feature_target(9, 391, 1, 599)
# insignificant feature
tar_feat3 <- create_feature_target(198, 202, 300, 300)
test_res <- test_features(tar_feat1[, 1], cbind(tar_feat1[, 2], tar_feat2[, 2],
                          tar_feat3[, 2]))
summary(test_res)
cut(test_res)

# real data example
# we will analyze only a subsample of a dataset to make analysis quicker
```

```
ids <- c(1L:100, 701L:800)
deg_seqs <- degenerate(human_cleave[ids, 1L:9],
                       list(`a` = c(1, 6, 8, 10, 11, 18),
                            `b` = c(2, 5, 13, 14, 16, 17, 19, 20),
                            `c` = c(3, 4, 7, 9, 12, 15)))

# positioned n-grams example
bigrams_pos <- count_ngrams(deg_seqs, 2, letters[1L:3], pos = TRUE)
test_features(human_cleave[ids, 10], bigrams_pos)

# unpositioned n-grams example, binarization required
bigrams_notpos <- count_ngrams(deg_seqs, 2, letters[1L:3], pos = TRUE)
test_features(human_cleave[ids, 10], binarize(bigrams_notpos))
```

`validate_encoding` *Validate encoding*

Description

Checks the structure of an encoding.

Usage

```
validate_encoding(x, u)
```

Arguments

x	encoding.
u	`integer`, `numeric` or `character` vector of all elements belonging to the encoding. See Details.

Details

The encoding is a list of groups to which elements of an alphabet should be reduced. All elements of the alphabet (all amino acids or all nucleotides) should appear in the encoding.

Value

`TRUE` if the `x` is a correctly reduced `u`, `FALSE` in any other cases.

See Also

`calc_ed`: calculate the encoding distance between two encodings. `encoding2df`: converts an encoding to a data frame.

Examples

```
enc1 = list(`1` = c("a", "t"),
            `2` = c("g", "c"))
# see if enc1 is the correctly reduced nucleotide (DNA) alphabet
validate_encoding(enc1, c("a", "c", "g", "t"))

# enc1 is not the RNA alphabet, so the results is FALSE
validate_encoding(enc1, c("a", "c", "g", "u"))

# validate_encoding works also on other notations
enc2 = list(a = c(1, 4),
            b = c(2, 3))
validate_encoding(enc2, 1L:4)
```

`write_encoding` *Write encodings to a file*

Description

Saves a list of encodings (or a single encoding to the file).

Usage

```
write_encoding(x, file = "")
```

Arguments

`x`	encoding or list of encodings.
`file`	ither a character string naming a file or a `connection` open for writing. `""` indicates output to the console.

Examples

```
aa1 = list(`1` = c("g", "a", "p", "v", "m", "l", "i"),
           `2` = c("k", "h"),
           `3` = c("d", "e"),
           `4` = c("f", "r", "w", "y", "s", "t", "c", "n", "q"))
write_encoding(aa1)
```

`write_fasta` *Write FASTA files*

Description

A lightweight tool to read nucleic or amino-acid sequences from a file in FASTA format.

Usage

```
write_fasta(seq, file, nchar = 80)
```

Arguments

`seq`	a list of sequences.
`file`	the name of the output file.
`nchar`	the number of characters per line.

See Also

`write.fasta`: heavier function for writing FASTA files.

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