Pse-in-One: a web server for generating various modes of pseudo components of DNA, RNA, and protein sequences

Manual of stand-alone program of Pse-in-One

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Home-page: http://bioinformatics.hitsz.edu.cn/Pse-in-One/







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1. Introduction of Pse-in-One

The **Pse-in-One** web server is able to generate totally 28 different modes of pseudo components for DNA, RNA, and protein sequences, including 14 modes for DNA sequences (**Table 1**), 6 modes for RNA sequences (**Table 2**), and 8 modes for protein sequences (**Table 3**).

To the best of our knowledge, **Pse-in-One** is so far the first web server that can generate all the possible pseudo components for DNA, RNA, and protein sequences, and even those defined by users themselves, and hence it is extremely flexible.

In order to handle large dataset, the stand-alone program of **Pse-in-One** is given, which is more powerful than the Pse-in-One web server, and will be introduced in the following parts of this manual.

2. Installation

The **Pse-in-One** package can be run on Linux, Mac, and Windows systems. Download the package from http://bioinformatics.hitsz.edu.cn/Pse-in-One/download and extract it to a directory, for example, "~/usr".

To execute the **Pse-in-One** in command line environment, navigate to the "~/usr/Pse-in-One-1.0/Pse-in-One" directory and you will find three python scripts, namely "kmer.py", "acc.py" and "pse.py". The "kmer.py" is used for calculating the modes in the category nucleic acid composition or amino acid composition; The "acc.py" is used for calculating the modes in autocorrelation category. The "pse.py" is used for calculating the modes in the category pseudo nucleotide composition or pseudo amino acid composition.

3. Input/Output formats

3.1. Input format

The input file should be a valid FASTA format that consists of a single initial line beginning with a greater-than symbol (">") in the first column, followed by lines of sequence data. The words right after the ">" symbol in the single initial line are optional and only used for the purpose of identification and description.

3.2. Output format

The output file formats support three choices that are suitable for downstream computational analyses, such as machine learning. The first and the default choice is the tab format. In this format, all data is separated by TABs. The second one is the LIBSVM's sparse data format. For this format, each line contains an instance and is ended by a '\n' character, like <label> <index1>:<value1> <index2>:<value2> The <label> is a category label of the sequence. The pair <index>:<value> gives a feature (attribute) value: <index> is an integer starting from 1 and <value> is a real number. The third output format is the csv format. This format is similar to the tab format. The only difference is the separation characters between data are commas.

3.3. Physicochemical Properties Selection

The Physicochemical Properties Selection file is a text file that contains a list of property names used for generating the modes in categories: autocorrelation, pseudo nucleotide composition/ pseudo amino acid composition. For example, if you want to use the "Rise", "Tilt" and "Shift" of DNA dinucleotide for calculating, the Physicochemical Properties Selection file should be written as follows:

Rise			
Tilt			
Shift			

After saving this file as "propChosen.txt" and specifying it using the command "-i propChosen.txt", or just "I propChosen.txt", the above three properties will be used in calculations. Meanwhile, you can also use the command "-a True" to select all the built-in physicochemical properties for the corresponding sequence type, which can be selected by using parameter DNA, RNA or PROTEIN.

The complete lists of physicochemical properties for DNA, RNA and protein sequences used in the stand-alone program are provided in **Table 4-8**.

3.4. User-defined Physicochemical Properties

In the user-defined physicochemical index files, each index should be represented in three lines. The first line must start with a greater-than symbol (">") in the first column. The words right after the ">" symbol in the single initial line are optional and only used for the purpose of identification and description of the index. The second line lists the names of the sequence compositions (i.e. amino acids, nucleotides, dinucleotides, or trinucleotides, etc), which should be sorted in the alphabet order, such as 'A' 'C' ... 'AA' 'AC'. All the elements in this line should be separated by TAB. The corresponding values of these sequence compositions are listed in the third line, which are separated by TAB.

For example, if you defined a physicochemical property "user_property", the user-defined physicochemical index file should be written as follows,

After saving this file as "user_defined.txt" and specifying it using the command "-e user_defined.txt", or just "E user_defined.txt", the properties defined by user will be used in calculations.

4. Commands

4.1 Command line parameters for kmer.py

	1 0
Options	Interpretations
inputfile	The input file in FASTA format.
outputfile The output file stored results.	
k	The k value of kmer.

{DNA, RNA, PROTEIN}	The sequence type.
-h,help	show this help message and exit.
-r {1,0}	Whether consider the reverse complement or not.
	1 means True, 0 means False. (default = 0)
-f {tab, svm, csv}	The output format. (default = tab)
	tab Simple format, delimited by TAB.
	svm The LIBSVM training data format.
	csv The format that can be loaded into a spreadsheet
	program.

4.2 Command line parameters for acc.py

Options	Interpretations
inputfile	The input file, in FASTA format.
outputfile	The output file stored results.
lag	The value of lag.
{DNA, RNA, PROTEIN}	The sequence type.
method	The method name of autocorrelation.
-h,help	show this help message and exit.
-i I	The index file user chosen.
-e E	The user-defined index file.
-a {True,False}	Choose all physicochemical indices or not. (default =
	False)
-f {tab,svm,csv}	The output format ($default = tab$).
	tab Simple format, delimited by TAB.
	svm The LIBSVM format.
	csv The format that can be loaded into a spreadsheet
	program.

4.3 Command line parameters for pse.py

Options	Interpretations
inputfile	The input file, in valid FASTA format.
outputfile	The outputfile stored results.
lamada	The value of lambda.
W	The value of weight.
{DNA, RNA, PROTEIN}	The sequence type.
method	The method name of pseudo components.
-h,help	show this help message and exit.
-i I	The index file user chosen.
-k K	The value of kmer, it works only with PseKNC method.
-e E	The user-defined index file, this parameter only needs to
	be set for PC-PseDNC-General, PC-PseTNC-General,
	SC-PseDNC-General, SC-PseTNC-General, PC-
	PseAAC-General or SC-PseAAC-General.
-a {True, False}	Choose all physicochemical indices or not. (default =

	False)
-f {tab, svm, csv}	The output format ($default = tab$).
	tab Simple format, delimited by TAB.
	svm The LIBSVM format.
	csv The format that can be loaded into a spreadsheet
	program.

4.4 Examples

For user's convenience, some examples of how to process a query sequence using command line are given below.

Example 1: Calculate the kmer composition feature vector of the query sequence and output the results in LIBSVM format.

```
kmer.py test.txt output_kmer.txt 2 DNA -f svm
```

After running the above command, the following results will be found in "output_kmer.txt" file.

0 1:0.023 2:0.034 3:0.053 4:0.023 5:0.045 6:0.086 7:0.143 8:0.06 9:0.049 10:0.15 11:0.124 12:0.049 13:0.015 14:0.064 15:0.053 16:0.03

Example 2: Calculate the auto covariance feature vector of the query sequence and output the results in LIBSVM format.

```
acc.py test.txt output_acc.txt 3 DNA TAC -a True -f svm
```

After running the above command, the following results will be found in "output_acc.txt" file.

0 1:-0.057 2:0.057 3:0.647 4:0.381 5:0.057 6:0.057 7:-0.051 8:-0.06 9:0.021 10:0.021 11:0.379 12:0.374 13:0.033 14:-0.011 15:0.413 16:0.019 17:-0.009 18:-0.009 19:-0.024 20:0.032 21:0.105 22:0.105 23:0.021 24:0.024 25:-0.008 26:-0.056 27:0.09 28:-0.088 29:-0.056 30:-0.056 31:-0.011 32:-0.008 33:-0.002 34:-0.002 35:-0.087 36:-0.085

Example 3: Calculate the PseDNC feature vector of the query sequence and output the results in CSV format.

```
pse.py test.txt output_pse.csv 3 0.2 DNA PseDNC
```

After running the above command, the following results will be found in "output_pse.csv" file.

0.01,0.016,0.024,0.01,0.021,0.04,0.066,0.028,0.023,0.069,0.057,0.023,0.007,0.02 9,0.024,0.014,0.217,0.152,0.17

Example 4: Calculate the PC-PseDNC-General feature vector of the query sequence using user-defined physicochemical index file and output the results in the CSV

format.

pse.py test.txt output_pse2.csv 3 0.2 DNA PC-PseDNC-General -e user_indices.txt -f csv

After running the above command, the following results will be found in "outut_pse2.csv" file.

0.011, 0.016, 0.025, 0.011, 0.021, 0.041, 0.068, 0.028, 0.023, 0.071, 0.059, 0.023, 0.007, 0.03, 0.025, 0.014, 0.213, 0.153, 0.161

The content of the file "test.txt" is listed as follow:

The content of the file "user_indices.txt" is listed as follow:

GGGCCGGACAATGAGAGTGTCCGCCTCC

>user_de	fined_pro	perty					
AA AC	AG AT	CA CC	CG CT	GA GC	GG GT	TA TC	TG TT
0.063	1.502	0.783	1.071	-1.376	0.063	-1.664	0.783 -
0.081	-0.081	0.063	1.502	-1.233	-0.081	-1.376	0.063

Table 1. 14 modes of DNA sequences calculated by PseDAC-General.

Category	Mode	Description
Nucleic acid	Kmer	Basic kmer (1)
Composition	RevKmer	Reverse complementary kmer (2,3)
	DAC	Dinucleotide-based auto covariance (4,5)
	DCC	Dinucleotide-based cross covariance (4,5)
Autocorrelation	DACC	Dinucleotide-based auto-cross covariance (4,5)
Autocorrelation	TAC	Trinucleotide-based auto covariance (5)
	TCC	Trinucleotide-based cross covariance (5)
	TACC	Trinucleotide-based auto-cross covariance (5)
	PseDNC	Pseudo dinucleotide composition (6)
	PseKNC	Pseudo k-tuple nucleotide composition (7,8)
	PC-PseDNC-	General parallel correlation pseudo dinucleotide
	General	composition (9)
Pseudo nucleotide	PC-PseTNC-	General parallel correlation pseudo trinucleotide
composition	General	composition (9)
•	SC-PseDNC-	General series correlation pseudo dinucleotide
	General	composition (9)
	SC-PseTNC-	General series correlation pseudo trinucleotide
	General	composition (9)

Table 2. 6 modes of RNA sequences calculated by PseRAC-General.

Category	Mode	Description
Nucleic acid composition	Kmer	Basic kmer (10)
Autocorrelation	DAC DCC DACC	Dinucleotide-based auto covariance (4,5,11) Dinucleotide-based cross covariance (4,5,11) Dinucleotide-based auto-cross covariance (4,5,11)
Pseudo nucleotide	PC-PseDNC-	General parallel correlation pseudo dinucleotide

composition	General SC-PseDNC-	composition (4,12) General series correlation pseudo dinucleotide
	General	composition (4,12)

Table 3. 8 modes of protein sequences calculated by PseAAC-General.

Category	Mode	Description
Amino acid composition	Kmer	Basic kmer (13)
Autocorrelation	AC CC ACC	Auto covariance (5,11) Cross covariance (5,11) Auto-cross covariance (5,11)
	PC-PseAAC	Parallel correlation pseudo amino acid composition (14)
Pseudo amino acid	SC-PseAAC	Series correlation pseudo amino acid composition (15)
composition	PC-PseAAC- General	General parallel correlation pseudo amino acid composition (14,16)
	SC-PseAAC- General	General series correlation pseudo amino acid composition (15,16)

Table 4. The names of the 148 physicochemical indices for dinucleotides.

Base stacking	Protein	B-DNA twist
	induced deformability	
Propeller twist	Duplex stability:(freeenergy)	Duplex tability(disruptenergy)
Protein DNA twist	Stabilising energy of Z-DNA	Aida_BA_transition
Breslauer_dS	Electron_interaction	Hartman_trans_free_energy
Lisser_BZ_transition	Polar_interaction	SantaLucia_dG
Sarai_flexibility	Stability	Stacking_energy
Sugimoto_dS	Watson-Crick_interaction	Twist
Shift	Slide	Rise
Twist stiffness	Tilt stiffness	Shift_rise
Twist_shift	Enthalpy1	Twist_twist
Shift2	Tilt3	Tilt1
Slide (DNA-protein complex)1	Tilt_shift	Twist_tilt
Roll_rise	Stacking energy	Stacking energy1
Propeller Twist	Roll11	Rise (DNA-protein complex)
Roll2	Roll3	Roll1
Slide_slide	Enthalpy	Shift_shift
Flexibility_slide	Minor Groove Distance	Rise (DNA-protein complex)1
Roll (DNA-protein complex)1	Entropy	Cytosine content
Major Groove Distance	Twist (DNA-protein complex)	Purine (AG) content
Tilt_slide	Major Groove Width	Major Groove Depth
Free energy6	Free energy7	Free energy4
Free energy3	Free energy1	Twist_roll
Flexibility_shift	Shift (DNA-protein complex)1	Thymine content
Tip	Keto (GT) content	Roll stiffness
Entropy1	Roll_slide	Slide (DNA-protein complex)
Twist2	Twist5	Twist4
Tilt (DNA-protein complex)1	Twist_slide	Minor Groove Depth
Persistance Length	Rise3	Shift stiffness
Slide3	Slide2	Slide1
Rise1	Rise stiffness	Mobility to bend towards minor
		•

		groove
Dinucleotide GC Content	A-philicity	Wedge
DNA denaturation	Bending stiffness	Free energy5
Breslauer_dG	Breslauer_dH	Shift (DNA-protein complex)
Helix-Coil_transition	Ivanov_BA_transition	Slide_rise
SantaLucia_dH	SantaLucia_dS	Minor Groove Width
Sugimoto_dG	Sugimoto_dH	Twist1
Tilt	Roll	Twist7
Clash Strength	Roll_roll	Roll (DNA-protein complex)
Adenine content	Direction	Probability contacting
		nucleosome core
Roll_shift	Shift_slide	Shift1
Tilt4	Tilt2	Free energy8
Twist (DNA-protein	Tilt_rise	Free energy2
complex)1		
Stacking energy2	Stacking energy3	Rise_rise
Tilt_tilt	Roll4	Tilt_roll
Minor Groove Size	GC content	Inclination
Slide stiffness	Melting Temperature1	Twist3
Tilt (DNA-protein complex)	Guanine content	Twist6
Major Groove Size	Twist_rise	Rise2
Melting Temperature	Free energy	Mobility to bend towards major
		groove

Table 5. The names of the 12 physicochemical indices for trinucleotides.

Bendability (DNAse)	Bendability (consensus)	Trinucleotide GC Content
Consensus_roll	Consensus-Rigid	Dnase I
MW-Daltons	MW-kg	Nucleosome
Nucleosome positioning	Dnase I-Rigid	Nucleosome-Rigid

Table 6. The names of the 6 physicochemical indices for dinucleotides.

Twist	Tilt	Roll	
Shift	Slide	Rise	

Table 7. The names of the 22 physicochemical indices for dinucleotides.

Shift (RNA)	Hydrophilicity (RNA)
Hydrophilicity (RNA)	GC content
Purine (AG) content	Keto (GT) content
Adenine content	Guanine content
Cytosine content	Thymine content
Slide (RNA)	Rise (RNA)
Tilt (RNA)	Roll (RNA)
Twist (RNA)	Stacking energy (RNA)
Enthalpy (RNA)	Entropy (RNA)
Free energy (RNA)	Free energy (RNA)
Enthalpy (RNA)	Entropy (RNA)

Table 8. The names of the 547 physicochemical indices for amino acids.

Hydrophobicity	Hydrophilicity	Mass	ANDN920101
ARGP820101	ARGP820102	ARGP820103	BEGF750101
BEGF750102	BEGF750103	BHAR880101	BIGC670101
BIOV880101	BIOV880102	BROC820101	BROC820102
BULH740101	BULH740102	BUNA790101	BUNA790102
BUNA790103	BURA740101	BURA740102	CHAM810101
CHAM820101	CHAM820102	CHAM830101	CHAM830102
CHAM830103	CHAM830104	CHAM830105	CHAM830106
CHAM830107	CHAM830108	CHOC750101	CHOC760101
CHOC760102	CHOC760103	CHOC760104	CHOP780101
CHOP780201	CHOP780202	CHOP780203	CHOP780204
CHOP780205	CHOP780206	CHOP780207	CHOP780208
CHOP780209	CHOP780210	CHOP780211	CHOP780212
CHOP780213	CHOP780214	CHOP780215	CHOP780216
CIDH920101	CIDH920102	CIDH920103	CIDH920104
CIDH920105	COHE430101	CRAJ730101	CRAJ730102
CRAJ730103	DAWD720101	DAYM780101	DAYM780201
DESM900101	DESM900102	EISD840101	EISD860101
EISD860102	EISD860103	FASG760101	FASG760102
FASG760103	FASG760104	FASG760105	FAUJ830101
FAUJ880101	FAUJ880102	FAUJ880103	FAUJ880104
FAUJ880105	FAUJ880106	FAUJ880107	FAUJ880108
FAUJ880109	FAUJ880110	FAUJ880111	FAUJ880112
FAUJ880113	FINA770101	FINA910101	FINA910102
FINA910103	FINA910104	GARJ730101	GEIM800101
GEIM800102	GEIM800103	GEIM800104	GEIM800105
GEIM800106	GEIM800107	GEIM800108	GEIM800109
GEIM800110	GEIM800111	GOLD730101	GOLD730102
GRAR740101	GRAR740102	GRAR740103	GUYH850101
HOPA770101	HOPT810101	HUTJ700101	HUTJ700102
HUTJ700103	ISOY800101	ISOY800102	ISOY800103
ISOY800104	ISOY800105	ISOY800106	ISOY800107
ISOY800108	JANJ780101	JANJ780102	JANJ780103
JANJ790101	JANJ790102	JOND750101	JOND750102
JOND920101	JOND920102	JUKT750101	JUNJ780101
KANM800101	KANM800102	KANM800103	KANM800104
KARP850101	KARP850102	KARP850103	KHAG800101
KLEP840101	KRIW710101	KRIW790101	KRIW790102
KRIW790103	KYTJ820101	LAWE840101	LEVM760101
LEVM760102	LEVM760103	LEVM760104	LEVM760105
LEVM760106	LEVM760107	LEVM780101	LEVM780102
LEVM780103	LEVM780104	LEVM780105	LEVM780106
LEWP710101	LIFS790101	LIFS790102	LIFS790103
MANP780101	MAXF760101	MAXF760102	MAXF760103
MAXF760104	MAXF760105	MAXF760106	MCMT640101
MEEJ800101	MEEJ800102	MEEJ810101	MEEJ810102
MEIH800101	MEIH800102	MEIH800103	MIYS850101
•			

NAGK730101	NAGK730102	NAGK730103	NAKH900101
NAKH900102	NAKH900103	NAKH900104	NAKH900105
NAKH900106	NAKH900107	NAKH900108	NAKH900109
NAKH900110	NAKH900111	NAKH900112	NAKH900113
NAKH920101	NAKH920102	NAKH920103	NAKH920104
NAKH920105	NAKH920106	NAKH920107	NAKH920108
NISK800101	NISK860101	NOZY710101	OOBM770101
OOBM770102	OOBM770103	OOBM770104	OOBM770105
OOBM850101	OOBM850102	OOBM850103	OOBM850104
OOBM850105	PALJ810101	PALJ810102	PALJ810103
PALJ810104	PALJ810105	PALJ810106	PALJ810107
PALJ810108	PALJ810109	PALJ810110	PALJ810111
PALJ810112	PALJ810113	PALJ810114	PALJ810115
PALJ810116	PARJ860101	PLIV810101	PONP800101
PONP800102	PONP800103	PONP800104	PONP800105
PONP800106	PONP800107	PONP800108	PRAM820101
PRAM820102	PRAM820103	PRAM900101	PRAM900102
PRAM900103	PRAM900104	PTIO830101	PTIO830102
QIAN880101	QIAN880102	QIAN880103	QIAN880104
QIAN880105	QIAN880106	QIAN880107	QIAN880108
QIAN880109	QIAN880110	QIAN880111	QIAN880112
QIAN880113	QIAN880114	QIAN880115	QIAN880116
QIAN880117	QIAN880118	QIAN880119	QIAN880120
QIAN880121	QIAN880122	QIAN880123	QIAN880124
QIAN880125	QIAN880126	QIAN880127	QIAN880128
QIAN880129	QIAN880130	QIAN880131	QIAN880132
QIAN880133	QIAN880134	QIAN880135	QIAN880136
QIAN880137	QIAN880138	QIAN880139	RACS770101
RACS770102	RACS770103	RACS820101	RACS820102
RACS820103	RACS820104	RACS820105	RACS820106
RACS820107	RACS820108	RACS820109	RACS820110
RACS820111	RACS820112	RACS820113	RACS820114
RADA880101	RADA880102	RADA880103	RADA880104
RADA880105	RADA880106	RADA880107	RADA880108
RICJ880101	RICJ880102	RICJ880103	RICJ880104
RICJ880105	RICJ880106	RICJ880107	RICJ880108
RICJ880109	RICJ880110	RICJ880111	RICJ880112
RICJ880113	RICJ880114	RICJ880115	RICJ880116
RICJ880117	ROBB760101	ROBB760102	ROBB760103
ROBB760104	ROBB760105	ROBB760106	ROBB760107
ROBB760108	ROBB760109	ROBB760110	ROBB760111
ROBB760112	ROBB760113	ROBB790101	ROSG850101
ROSG850102	ROSM880101	ROSM880102	ROSM880103
SIMZ760101	SNEP660101	SNEP660102	SNEP660103
SNEP660104	SUEM840101	SUEM840102	SWER830101
TANS770101	TANS770102	TANS770103	TANS770104
TANS770105	TANS770106	TANS770107	TANS770108
TANS770109	TANS770110	VASM830101	VASM830102
VASM830103	VELV850101	VENT840101	VHEG790101

WARP780101	WEBA780101	WERD780101	WERD780102
WERD780103	WERD780104	WOEC730101	WOLR810101
WOLS870101	WOLS870102	WOLS870103	YUTK870101
YUTK870102	YUTK870103	YUTK870104	ZASB820101
ZIMJ680101	ZIMJ680102	ZIMJ680103	ZIMJ680104
ZIMJ680105	AURR980101	AURR980102	AURR980103
AURR980104	AURR980105	AURR980106	AURR980107
AURR980108	AURR980109	AURR980110	AURR980111
AURR980112	AURR980113	AURR980114	AURR980115
AURR980116	AURR980117	AURR980118	AURR980119
AURR980120	ONEK900101	ONEK900102	VINM940101
VINM940102	VINM940103	VINM940104	MUNV940101
MUNV940102	MUNV940103	MUNV940104	MUNV940105
WIMW960101	KIMC930101	MONM990101	BLAM930101
PARS000101	PARS000102	KUMS000101	KUMS000102
KUMS000103	KUMS000104	TAKK010101	FODM020101
NADH010101	NADH010102	NADH010103	NADH010104
NADH010105	NADH010106	NADH010107	MONM990201
KOEP990101	KOEP990102	CEDJ970101	CEDJ970102
CEDJ970103	CEDJ970104	CEDJ970105	FUKS010101
FUKS010102	FUKS010103	FUKS010104	FUKS010105
FUKS010106	FUKS010107	FUKS010108	FUKS010109
FUKS010110	FUKS010111	FUKS010112	AVBF000101
AVBF000102	AVBF000103	AVBF000104	AVBF000105
AVBF000106	AVBF000107	AVBF000108	AVBF000109
YANJ020101	MITS020101	TSAJ990101	TSAJ990102
COSI940101	PONP930101	WILM950101	WILM950102
WILM950103	WILM950104	KUHL950101	GUOD860101
JURD980101	BASU050101	BASU050102	BASU050103
SUYM030101	PUNT030101	PUNT030102	GEOR030101
GEOR030102	GEOR030103	GEOR030104	GEOR030105
GEOR030106	GEOR030107	GEOR030108	GEOR030109
ZHOH040101	ZHOH040102	ZHOH040103	BAEK050101
HARY940101	PONJ960101	DIGM050101	WOLR790101
OLSK800101	KIDA850101	GUYH850102	GUYH850103
GUYH850104	GUYH850105	ROSM880104	ROSM880105
JACR890101	COWR900101	BLAS910101	CASG920101
CORJ870101	CORJ870102	CORJ870103	CORJ870104
CORJ870105	CORJ870106	CORJ870107	CORJ870108
MIYS990101	MIYS990102	MIYS990103	MIYS990104
MIYS990105	ENGD860101	FASG890101	
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