

# Package ‘affypdnn’

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**Title** Probe Dependent Nearest Neighbours (PDNN) for the affy package

**Author** H. Bjorn Nielsen and Laurent Gautier (Many thanks to Li Zhang early communications about the existence of the PDNN program and related publications).

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**Depends** R (>= 2.13.0), affy (>= 1.5)

**Suggests** affydata, hgu95av2probe

**Description** The package contains functions to perform the PDNN method described by Li Zhang et al.

**License** LGPL

**biocViews** OneChannel, Microarray, Preprocessing

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 expressopdnn

*Position Dependant Nearest Neighbors model for affy*


---

## Description

A wrapper to perform the PDNN method.

## Usage

```
pdnn.scalevalue.exprSet(eset, scale.to=500)
expressopdnn(abatch,
  # background correction
  bg.correct = FALSE,
  bgcorrect.method = NULL,
  bgcorrect.param = list(),
  # normalize
  normalize = FALSE,
  normalize.method = NULL,
  normalize.param = list(),

  pmcorrect.method = c("pdnn", "pdnnpredict"),

  # pdnn
  findparams.param = list(),
  # expression values
  summary.subset = NULL,
  # PDNN expression values scaling
  eset.normalize = TRUE,
  scale.to = 500,
  # misc.
  verbose = TRUE)
```

## Arguments

abatch	object of <a href="#">AffyBatch-class</a> .
bg.correct	a boolean to express whether background correction is wanted or not.
bgcorrect.method	the name of the background adjustment method.
bgcorrect.param	a list of parameters for bgcorrect.method (if needed/wanted).
eset	an object of <a href="#">ExpressionSet-class</a> .
normalize	normalization step wished or not.
normalize.method	the normalization method to use.
normalize.param	a list of parameters to be passed to the normalization method (if wanted).
pmcorrect.method	the name of the PM adjustment method (only two choices here, default to 'pdnn').

<code>findparams.param</code>	a list of parameters to be passed to <code>find.params.pdnn</code> .
<code>eset.normalize</code>	is any normalization step on expression values to be performed.
<code>scale.to</code>	a value to scale against.
<code>summary.subset</code>	a list of 'affyids'. If NULL, then an expression summary value is computed for everything on the chip.
<code>verbose</code>	logical value. If TRUE it writes out some messages.

## Details

`expressopdnn` is very similar to [expresso](#). It is mainly a wrapper around the pre-processing steps 'background correction', 'normalization', 'perfect match correction' and the PDNN method to compute expression values (see the first reference for more details about the preprocessing steps and the second reference for further details about the PDNN method).

The wrapper `expresso` has no way to handle easily the computation of chip-wide results that have to be used during the `computeExprSet` step. An easy way to overcome this was to write this simple wrapper.

`pdnn.scalevalue` is performed after the expression values have computed to somehow 'normalize' the values between different chips. When setting `normalize` to TRUE this step might be considered unnecessary (and the `eset.normalize` set to FALSE).

## Value

An object of [ExpressionSet-class](#), with an attribute `pps.warnings` as returned by the method [computeExprSet](#).

## See Also

[expresso](#) and [generateExprVal.method.pdnn](#)

## Examples

```
## load pre-computed parameters
data(hgu95av2.pdnn.params)

library(affydata)
data(Dilution)

## one CEL to go faster
afbatch <- Dilution[, 1]

## Take only few IDs (the 10 first)
ids <- ls(getCdfInfo(afbatch))[1:10]
eset <- expressopdnn(afbatch, bg.correct=FALSE,
                    normalize=FALSE,
                    findparams.param=list(params.chiptype=hgu95av2.pdnn.params,
                                           give.warnings=FALSE),
                    summary.subset=ids)
```

---

find.params.pdnn      *A function to find the experiment specific PDNN parameters*

---

## Description

A function to find the parameters specific to the chips in an AffyBatch object.

## Usage

```
find.params.pdnn(abatch, params.chiptype, optim.method = "BFGS", verbose = TRUE, give.warnings=TRUE)
```

## Arguments

abatch	an instance of <a href="#">AffyBatch-class</a> .
params.chiptype	chip-type specific parameters (see details)
optim.method	method for the optimization function <a href="#">optim</a> . When FALSE, a steepest-descent method of our own is used.
verbose	verbosity (TRUE or FALSE)
give.warnings	report probeset IDs in the abatch that could not be found in the params.chiptype

## Details

This function fits PDNN parameters that are specific to experimental values. The parameters common to all the chips of a certain type are returned by the function [pdnn.params.chiptype](#). If NULL, the parameter files included in the package will be used whenever possible...

## Value

A list of

lambda	The lambda's
Bs	The B's
Ns	The N's
Fs	The F's

## References

Li Zhang, Michael F. Miles and Kenneth D. Aldape - A model of molecular interactions on short oligonucleotide arrays, 2003, Nature Biotech., vol. 21, n.7

## See Also

[pdnn.params.chiptype](#), [generateExprVal.method.pdnn](#)

**Examples**

```
## load a chip-specific parameter file
## (as returned by the function pdnn.params.chiptype)
data(hgu95av2.pdnn.params)

## load experimental data
library(affydata)
data(Dilution)

## one CEL to go faster
afbatches <- Dilution[, 1]
params <- find.params.pdnn(afbatches, hgu95av2.pdnn.params, optim.method =
FALSE, give.warnings=FALSE)
```

---

```
generateExprVal.method.pdnn
```

*Compute PM correction and summary expression value*

---

**Description**

Computes PM correction and summary expression value with PDNN method.

**Usage**

```
pmcorrect.pdnn(object, params, gene=NULL, gene.i=NULL,
               params.chiptype=NULL, outlierlim=3, callingFromExpresso=FALSE)
pmcorrect.pdnnpredict(object, params, gene=NULL, gene.i=NULL,
                      params.chiptype=NULL, outlierlim=3, callingFromExpresso=FALSE)
generateExprVal.method.pdnn(probes, params)
```

**Arguments**

object	object of <a href="#">ProbeSet</a> .
probes	matrix of PM-corrected signals (should be coming out of <code>pmcorrect.pdnn</code> ).
params	experiments specific parameters.
gene	gene (probe set) ID (from which the <code>gene.i</code> would be derived).
gene.i	gene index (see details).
params.chiptype	chip-specific parameters.
outlierlim	threshold for tagging a probe as an outlier.
callingFromExpresso	is the function called through <code>expresso</code> . DO NOT play with that.

**Details**

Only one of `gene`, `gene.i` should be specified. For most the users, this is `gene`. `pmcorrect.pdnn` and `pmcorrect.pdnnpredict` return what is called GSB and GSB + NSB + B in the paper by Zhang Li and collaborators.

**Value**

pmcorrect.pdnn and pmcorrect.pdnnpredict return a matrix (one row per probe, one column per chip) with attributes attached. generateExprVal returns a list:

```
exprs           expression values
se.exprs       se expr. val.
```

**See Also**

[pdnn.params.chiptype](#)

**Examples**

```
data(hgu95av2.pdnn.params)
library(affydata)
data(Dilution)

## only one CEL to go faster
abatch <- Dilution[, 1]

## get the chip specific parameters
params <- find.params.pdnn(abatch, hgu95av2.pdnn.params)

## The thrill part: do we get like in the Figure 1-a of the reference ?
par(mfrow=c(2,2))
##ppset.name <- sample(featureNames(abatch), 2)
ppset.name <- c("41206_r_at", "31620_at")
ppset <- probeset(abatch, ppset.name)
for (i in 1:2) {
  ##ppset[[i]] <- transform(ppset[[i]], fun=log) # take the log as they do
  probes.pdnn <- pmcorrect.pdnnpredict(ppset[[i]], params,
                                     params.chiptype=hgu95av2.pdnn.params)

  ##probes.pdnn <- log(probes.pdnn)
  plot(ppset[[i]], main=paste(ppset.name[i], "\n(raw intensities)"))
  matplotProbesPDNN(probes.pdnn, main=paste(ppset.name[i], "\n(predicted intensities)"))
}

## pick the 50 first probeset IDs
## (to go faster)
ids <- featureNames(abatch)[1:100]

## compute the expression set (object of class 'ExpressionSet')
eset <- computeExprSet(abatch, pmcorrect.method="pdnn",
                      summary.method="pdnn", ids=ids,
                      summary.param = list(params, params.chiptype=hgu95av2.pdnn.params))
```

---

hgu133a.pdnn.params    *Chip-type specific data*

---

**Description**

Chip-type specific data structure.

**Usage**

```
data(hgu95av2.pdnn.params)
```

**Format**

The format is a list:

**Eg** environment (one entry per dinucleotide)

**Wg** numerical vector.

**En** environment (one entry per dinucleotide)

**Wn** numerical vector.

**gene.Sn** list (one entry per affyID)

**gene.Sg** list (one entry per affyID)

**gene.xy** list (one entry per affyID)

**params.gene** environment

**Details**

These chip-specific data structures are generated from the data files made available by the author of the PDNN paper (see the section source). They are stored as data to save some computation time. The data structures were made using the function `pdnn.params.chiptype`. The data files are included in the the directory 'data' of the package.

**Note**

To lower the size of the package, the only chip-specific data structures included in the package is the one for HG-U95Av2.

**Source**

Li Zhang, Michael F. Miles and Kenneth D. Aldape - A model of molecular interactions on short oligonucleotide arrays, 2003, Nature Biotech., vol. 21, n.7

**Examples**

```
## give the path the original energy parameter files included in the package
list.files(system.file("exampleData", package="affypdnn"),
           "^pdnn-energy-parameter_", full.names=TRUE)
```

---

matplotProbesPDNN

*Plot the PDNN computed probe intensities*


---

**Description**

Plot the probe intensities as computed by 'pmcorrect.pdnn' or 'pmcorrect.pdnnpredict'

**Usage**

```
matplotProbesPDNN(x, type="l", ...)
```

**Arguments**

x a matrix (and attributes) as returned by `pmcorrect.pdnn` or `pmcorrect.pdnnpredict`.  
 type type of plot (same as in `matplot`)  
 ... optional arguments to be passed to `matplot`

**Details**

The crosses are the probe intensities which are considered ‘ok’ by the outlier detection part of the algorithm, while the circles are the ones considered ‘outliers’

**Value**

Only used for its side-effect.

**See Also**

[pmcorrect.pdnn](#) and [pmcorrect.pdnnpredict](#)

**Examples**

```
# see 'pmcorrect.pdnn'
```

---

<code>params.dilution</code>	<i>Parameters for the Dilution dataset</i>
------------------------------	--

---

**Description**

PDNN parameters for the Dilution dataset

**Usage**

```
data(params.dilution)
```

**Format**

The format is: List of 6 \$ lambda :List of 12625 (probesets) ... \$ Bs : num [1:4] 111.9 57.3 120.5 50.1 \$ Ns : num [1:4] 2967 2998 2992 2999 \$ Fs : num [1:4] 0.607 0.662 0.600 0.656 \$ names.abatch: chr [1:12625] "1000\\_at" "1001\\_at" "1002\\_f\\_at" ... \$ names.i : int [1:12625] 1 2 3 4 5 6 7 8 9 10 ...

**Details**

These data are provided to reduce the time needed to run the vignette.

**Examples**

```
data(params.dilution)
```



---

pdnn.params.chiptype *A function to fit PDNN parameters*

---

### Description

A function to fit PDNN parameters that are chip-type specific

### Usage

```
pdnn.params.chiptype(energy.param.file, probes.file = NULL, probes.pack= NULL,
                    probes.data.frame = NULL,
                    seq.name, x.name, y.name, affyid.name, verbose = TRUE)
```

### Arguments

energy.param.file	Path to the energy data file (see details)
probes.file	Path to the probe files (see details)
probes.pack	Name of the probe pack (see details)
probes.data.frame	A data.frame
seq.name, x.name, y.name, affyid.name	The names of the columns in the data.frame from probes.pack or probes.file for the probe sequences, the X positions, the Y positions and the probe set ID respectively
verbose	verbosity (TRUE or FALSE)

### Details

The parameters probes.file, probes.pack and probes.data.frame are mutually exclusive. The function fits PDNN parameters that are specific to chip-types (hence specific to the probe sequences). It requires data files like the one found on Li Zhang's web page: (<http://odin.mdacc.tmc.edu/~zhangli/PerfectM>). This should be computed once for all for a given chip type. Computed values for the chips are included in the package. This allows 'automagic' use of them when these chips types are used (as done in the function [expresspdnn](#)).

### Value

A list of:

Eg	environment. One entry per dinucleotide.
Wg	numerical vector
En	environment. One entry per dinucleotide.
Wn	numerical vector
params.gene	environment. One entry per gene, each entry is a list of elements Sg, Sn, xy and gene.i

### warning

The X and Y positions in the data.frame are expected to be original ones in the Affymetrix files (starting at zero. They are offset by one within this function.

**See Also**

[find.params.pdnn](#)

**Examples**

```
if (interactive()) {  
  energy.file <- system.file("exampleData", "pdnn-energy-parameter_hg-u95av2.txt", package="affypdnn")  
  
  params.chiptype <- pdnn.params.chiptype(energy.file, probes.pack="hgu95av2probe")  
}
```

---

transform.ProbeSet     *A function to transform a ProbeSet*

---

**Description**

A function to transform the PMs and MMs in a ProbeSet.

**Usage**

```
## S3 method for class 'ProbeSet'  
transform(`_data`, fun = I, ...)
```

**Arguments**

<code>_data</code>	object of <a href="#">ProbeSet-class</a> .
<code>fun</code>	a function. The identity function by default.
<code>...</code>	optional arguments for fun.

**Details**

The function fun is applied to the slots pm and mm. The function vsnh in the package vsn is a recommended argument for fun.

**Value**

An object of class ProbeSet.

**Note**

This function should make to the package affy for the version 1.4.x.

**Author(s)**

Laurent

**Examples**

```
library(affydata)

data(Dilution)

ppset.name <- sample(featureNames(Dilution), 1)
ppset <- probeset(Dilution, ppset.name)[[1]]
ppset.log <- transform(ppset, fun=log)

par(mfrow=c(1,2))
plot(ppset)
plot(ppset.log)
```

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