

Package ‘magp’

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Title Mapping-Based Additive Gaussian Process Models

Version 0.8.0

Description Fits mapping-based additive Gaussian process models for experiments in which each component has both a quantitative level and a position in an ordered sequence. Two model structures are available: a compact two-dimensional mapping and a full mapping with one fewer dimension than the number of components. Both models support parameter estimation, point prediction, and plug-in predictive uncertainty. Input checks validate the sequence data and apply consistent scaling to the quantitative inputs. Computationally intensive covariance and gradient calculations are implemented in C++ with 'Rcpp'. The model was introduced by Xiao et al. (2024) <[doi:10.1080/01621459.2022.2123335](https://doi.org/10.1080/01621459.2022.2123335)>.

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Author Tony Wang [aut, cre, cph],
Qian Xiao [aut, cph],
Yaping Wang [cph],
Abhyuday Mandal [cph],
Xinwei Deng [cph]

Maintainer Tony Wang <wangtony883@gmail.com>

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magp2d_fit	<i>Fit a MaGP model with a two-dimensional sequence map</i>
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Description

Fits an additive Gaussian process for data that combine component amounts with a component order. Sequence positions are represented by points in a compact two-dimensional latent map.

Usage

```
magp2d_fit(  
  X,  
  y = NULL,  
  q = NULL,  
  tau = 0.001,  
  maxeval = 500,  
  xtol_rel = 1e-05,  
  lb_sigma = 10,  
  ub_sigma = 1000,  
  lb_theta = 0.5,  
  ub_theta = 1000,  
  lb_delta = -1,  
  ub_delta = 1,  
  seed = NULL  
)
```

Arguments

- X A numeric matrix or data frame. The first q input columns contain quantitative levels and the next q columns contain sequence positions. Each sequence row must be a permutation of 1 : q. A column named y may be included as the response.
- y An optional numeric response vector. It may be omitted when X contains a response column named y.
- q The number of components. It is inferred from the number of input columns when omitted. The two-dimensional model requires at least three components; the full model requires at least two.

tau	A fixed nonnegative nugget variance added to the covariance diagonal.
maxeval	Maximum number of objective evaluations used by nloptr.
xtol_rel	Relative parameter tolerance used by nloptr.
lb_sigma, ub_sigma	Lower and upper bounds for the additive variance parameters.
lb_theta, ub_theta	Lower and upper bounds for the quantitative correlation parameters.
lb_delta, ub_delta	Lower and upper bounds for the mapping parameters.
seed	An optional nonnegative integer used to generate the initial parameter vector.

Details

The covariance is a sum of component-specific terms. Each term combines the distance between two quantitative levels with the distance between their mapped sequence positions. The variance, correlation, and mapping parameters are estimated together with bounded optimization.

Quantitative columns outside $[0, 1]$ are transformed with column-wise min-max scaling. Their training ranges are stored in the fitted object and reused for prediction. Columns already in $[0, 1]$ are left unchanged.

Value

An object of class magp2d.

Examples

```
train <- read.table(
  system.file("extdata", "example_train.txt", package = "magp"),
  header = TRUE
)
fit <- magp2d_fit(train, seed = 1)
fit
```

magp2d_rmse

Calculate root-mean-squared prediction error

Description

Calculates the root-mean-squared error between predicted and observed values.

Usage

```
magp2d_rmse(pred, actual)
```

Arguments

pred	Numeric vector of predictions.
actual	Numeric vector of observed values with the same length as pred.

Value

A single nonnegative numeric value.

magpfull_fit	<i>Fit a MaGP model with a full sequence map</i>
--------------	--

Description

Fits the quantitative-sequence model with $q - 1$ latent mapping dimensions, giving the sequence positions a less constrained coordinate representation.

Usage

```
magpfull_fit(
  X,
  y = NULL,
  q = NULL,
  tau = 0.001,
  maxeval = 500,
  xtol_rel = 1e-05,
  lb_sigma = 10,
  ub_sigma = 1000,
  lb_theta = 0.5,
  ub_theta = 1000,
  lb_delta = -1,
  ub_delta = 1,
  seed = NULL
)
```

Arguments

X	A numeric matrix or data frame. The first q input columns contain quantitative levels and the next q columns contain sequence positions. Each sequence row must be a permutation of $1 : q$. A column named <code>y</code> may be included as the response.
y	An optional numeric response vector. It may be omitted when <code>X</code> contains a response column named <code>y</code> .
q	The number of components. It is inferred from the number of input columns when omitted. The two-dimensional model requires at least three components; the full model requires at least two.
tau	A fixed nonnegative nugget variance added to the covariance diagonal.

maxeval	Maximum number of objective evaluations used by nloptr.
xtol_rel	Relative parameter tolerance used by nloptr.
lb_sigma, ub_sigma	Lower and upper bounds for the additive variance parameters.
lb_theta, ub_theta	Lower and upper bounds for the quantitative correlation parameters.
lb_delta, ub_delta	Lower and upper bounds for the mapping parameters.
seed	An optional nonnegative integer used to generate the initial parameter vector.

Details

The data layout, quantitative scaling, and covariance construction are the same as in [magp2d_fit\(\)](#). The difference is the number of latent coordinates used to represent the sequence positions.

Value

An object of class magpfull.

Examples

```
train <- read.table(
  system.file("extdata", "example_train.txt", package = "magp"),
  header = TRUE
)
fit <- magpfull_fit(train, seed = 1)
fit
```

predict.magp	<i>Predict outcomes from a fitted MaGP model</i>
--------------	--

Description

Returns predictions for new quantitative-sequence inputs. Plug-in standard errors and variances can be returned with the predictions.

Usage

```
## S3 method for class 'magp2d'
predict(
  object,
  newdata,
  se.fit = FALSE,
  type = c("script", "response", "latent"),
  ...
)
```

```
## S3 method for class 'magnfull'
predict(
  object,
  newdata,
  se.fit = FALSE,
  type = c("script", "response", "latent"),
  ...
)
```

Arguments

object	A fitted magn2d or magnfull object.
newdata	A numeric matrix or data frame with the same quantitative and sequence inputs used for fitting. A response column named y is ignored.
se.fit	Logical; if TRUE, return predictive standard errors and variances in addition to fitted values.
type	Prediction convention. "script" uses the fitted training-row convention when newdata exactly matches a training row. "response" includes the nugget variance for a future response, and "latent" returns uncertainty for the noise-free surface.
...	Additional arguments, currently unused.

Value

If `se.fit = FALSE`, a numeric vector of predictions. Otherwise, a list with components `fit`, `se.fit`, `variance`, and `type`.

Examples

```
train <- read.table(
  system.file("extdata", "example_train.txt", package = "magn"),
  header = TRUE
)
test <- read.table(
  system.file("extdata", "example_test.txt", package = "magn"),
  header = TRUE
)
fit <- magn2d_fit(train, seed = 1)
predict(fit, test[1:3, ], se.fit = TRUE, type = "response")
```

print.magp2d	<i>Summarize a fitted two-dimensional MaGP model</i>
--------------	--

Description

Prints the model size, nugget variance, fitted mean, objective value, and optimizer status.

Usage

```
## S3 method for class 'magp2d'  
print(x, ...)
```

Arguments

x	A magp2d model returned by magp2d_fit() .
...	Unused.

Value

x, invisibly.

print.magpfull	<i>Summarize a fitted full-mapping MaGP model</i>
----------------	---

Description

Prints the mapping dimension, model size, nugget variance, fitted mean, objective value, and optimizer status.

Usage

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

Arguments

x	A magpfull model returned by magpfull_fit() .
...	Unused.

Value

x, invisibly.

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