OpenTURNS release highlights : the new Gaussian Process API

S.Haddad (Airbus Central R&T)

User Day #18, June 13th 2025, EDF Lab

Contents

Kriging implementation: basic example

```python
import openturns as ot
...
# Call kriging
kriging_algo = ot.KrigingAlgorithm(X_train, Y_train, covarianceModel, b
kriging_algo.run()
# Get the result
kriging_result = kriging_algo.getResult()
# Post-processing
func = kriging_result.getMetaModel()
# Conditional variance
cond_var = kriging_result.getConditionalVariance(new_X)
```

First remarks:

- `KrigingAlgorithm` handles the E2E computation,
- Post-processing methods handled by result structures;

Kriging implementation: change some parameters

```python
import openturns as ot

# Set optimizer
ot.ResourceMap.SetAsString(
  "GeneralLinearModelAlgorithm-DefaultOptimizationAlgorithm", "Cobyla")
ot.ResourceMap.SetAsScalar(
  "GeneralLinearModelAlgorithm-DefaultOptimizationLowerBound", 0)
ot.ResourceMap.SetAsScalar(
  "GeneralLinearModelAlgorithm-DefaultOptimizationUpperBound", 2)
ot.ResourceMap.SetAsString(
  "KrigingAlgorithm-LinearAlgebra", "LAPACK")
#ot.ResourceMap.SetAsString(
#  "GeneralLinearModelAlgorithm-LinearAlgebra", "LAPACK")


...
# Call kriging
kriging_algo = ot.KrigingAlgorithm(X_train, Y_train, covarianceModel, b
kriging_algo.run()
# Get the result
```

In a nutshell

`KrigingAlgorithm` is used to fit a Kriging model (aka Gaussian Process Regression), relying on a 2-steps procedure :

- `GeneralLinearModelAlgorithm`: allowing the parametric estimation of a Gaussian Process,
- `KrigingAlgorithm`: conditioning the Gaussian Process;

$\longrightarrow$ `KrigingAlgorithm.run` calibrate a Gaussian Process

- `ResourceMap` keys duplicate,
- Sequential Kriging hard to handle (example for `EGO`);

Our wishes

- Trigger explicitly the parameters fitting,
- Perform the conditioning,
- Enrich the API with missing features (such as "known trend"),
- Build as much post-processing functions as needed;

New API for Gaussian Process Regression

The new API defines the following classes (in the `experimental` submodule):

- `GaussianProcessFitter`: Fitting the Gaussian Process (explicitly),
- `GaussianProcessFitterResult`: result class of a parametric Gaussian Process fitting,
- `GaussianProcessRegression`: conditioning the Gaussian Process,
- `GaussianProcessRegressionResult`: result class of a conditional Gaussian Process fitting,
- `GaussianProcessRandomVector`: generate Gaussian Process realizations,
- `GaussianProcessConditionalCovariance`: Post-processing Gaussian Process;

```
# Call fitter
fitter_algo = otexp.GaussianProcessFitter(X_train, Y_train, covarianceM
fitter_algo.run()
fitter_result = fitter_algo.getResult()
# Conditioning part using the fit result
gpr_algo = otexp.GaussianProcessRegression(fitter_result)
gpr_algo.run()
gpr_result = gpr_algo.getResult()
gpr_metamodel = gpr_result.getMetaModel()
```

New feature : known trend

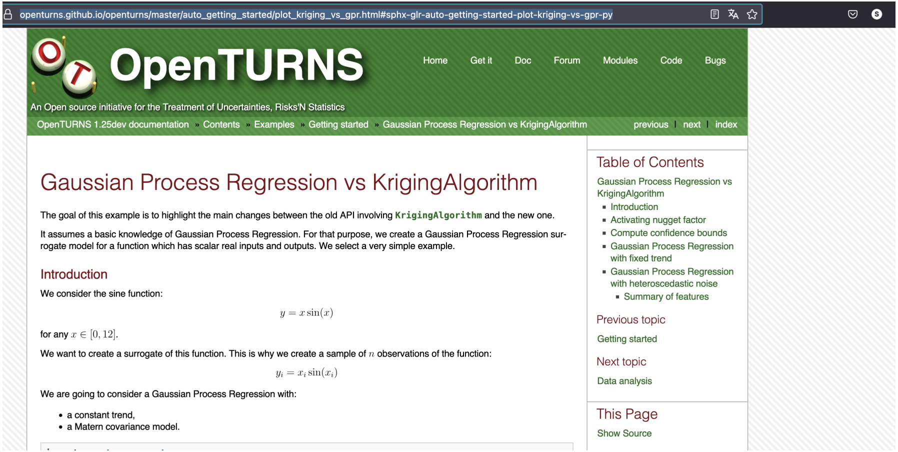
```
# trend function
trend_function = ot.SymbolicFunction("x", "-3.1710410094572903")
# Covariance
scale = [4.51669]
amplitude = [8.648]
covariance_opt = ot.MaternModel(scale, amplitude, 1.5)
# Conditioning part using the data
gpr_algo_noopt = otexp.GaussianProcessRegression(x_train, y_train, cova
gpr_algo_noopt.run()
gpr_result_no_opt = gpr_algo_noopt.getResult()
gpr_nopt_Metamodel = gpr_result_no_opt.getMetaModel()
```

Post-processing : conditional covariance

```
# Call fitter
fitter_algo = otexp.GaussianProcessFitter(X_train, Y_train, covarianceM
fitter_algo.run()
fitter_result = fitter_algo.getResult()
# Conditioning part using the fit result
gpr_algo = otexp.GaussianProcessRegression(fitter_result)
gpr_algo.run()
gpr_result = gpr_algo.getResult()
# Conditional covariance
gpcc = otexp.GaussianProcessConditionalCovariance(gpr_result)
cond_var = gpcc.getConditionalVariance(new_X)
```

Kriging vs Gaussian Process

Reach out here to learn more !



openturns.github.io/openturns/master/auto_getting_started/plot_kriging_vs_gpr.html#sphx-glr-auto-getting-started-plot-kriging-vs-gpr-py

OpenTURNS

Home Get it Doc Forum Modules Code Bugs

An Open source initiative for the Treatment of Uncertainties, Risks'N Statistics

OpenTURNS 1.25dev documentation » Contents » Examples » Getting started » Gaussian Process Regression vs KrigingAlgorithm

previous | next | index

Gaussian Process Regression vs KrigingAlgorithm

The goal of this example is to highlight the main changes between the old API involving `KrigingAlgorithm` and the new one.

It assumes a basic knowledge of Gaussian Process Regression. For that purpose, we create a Gaussian Process Regression surrogate model for a function which has scalar real inputs and outputs. We select a very simple example.

Introduction

We consider the sine function:

$$y = x \sin(x)$$

for any $x \in [0, 12]$.

We want to create a surrogate of this function. This is why we create a sample of n observations of the function:

$$y_i = x_i \sin(x_i)$$

We are going to consider a Gaussian Process Regression with:

- a constant trend,
- a Matern covariance model.

Table of Contents

Previous topic

Getting started

Next topic

Data analysis

This Page

Show Source

Summary

Feature	OpenTURNS 1.24	New API
`Optimisation`	`TNC`	`Cobyla`
`Heteroscedasticity`	`KrigingAlgorithm.setNoise`	`Not implemented`
`Nugget factor est`	`CovModel`	`CovModel`
`Known trend`	`Not implemented`	`Implemented`
`Conditional covariance`	`KrigingResult`	`GPCC*`

*GPCC: GaussianProcessConditionalCovariance

Integration within OpenTURNS

List of classes supporting the new API:

- `EfficientGlobalOptimization`: rely on `GaussianProcessRegressionResult`,
- `ConditionedGaussianProcess`: rely on `GaussianProcessRegressionResult`

Remark : these classes are now part of the experimental submodule!
In parallel, all examples involving Kriging are progressively moving to the new API !

Outlook

2025-2026 work

- Finalize migration of the examples to the new API,
- Algebra of covariance models,
- Analytical gradient of covariance models,
- Integration into the existing algorithms,
- Cross-validation methods,
- Sequential algorithms,

END

Thank you for your attention!
Any questions?