Low rank tensor approximation in OpenTURNS

J. Schueller

Phimeca

EDF, 2016-06-21





Plan

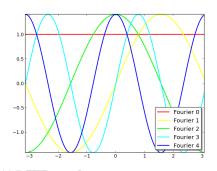
- Non-polynomial basis
- Canonical tensor



Fourier series

Fourier series

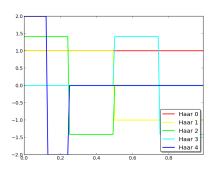
$$\begin{array}{rcl} \psi_0(x) & = & 1 \\ \psi_{2k+1}(x) & = & \sqrt{2}\sin(kx) \\ \psi_{2k+2}(x) & = & \sqrt{2}\cos(kx) \end{array}$$



Haar wavelets

Haar wavelets

$$\begin{array}{rcl} \psi_0(x) & = & \mathbbm{1}_{[0,1]}(x) \\ \psi_n(x) & = & \frac{1}{2^{j/2}} \left[\mathbbm{1}_{\left[\frac{k}{2^j}, \frac{k+1/2}{2^j}\right]}(x) - \mathbbm{1}_{\left[\frac{k+1/2}{2^j}, \frac{k+1}{2^j}\right]}(x) \right] \end{array}$$



Usage

```
In Python...
```

```
# as a regular function
family = ot.FourierSeriesFactory()
family = ot.HaarWaveletFactory()

for i in range(5):
    f = family.build(i)
    d = f.draw(xmin, xmax, 100)
```



Functional chaos tensorization

Tensorization

Functional chaos decomposition

$$Y \equiv h(\underline{X}) = \sum_{j=0}^{\infty} a_j \, \psi_j(\underline{X})$$

upon tensorized basis

$$\psi_{\alpha}(\underline{x}) \equiv \pi_{\alpha_1}^{(1)}(x_1) \times \cdots \times \pi_{\alpha_d}^{(d)}(x_d)$$

multi-indices notation

$$\alpha \equiv \{\alpha_1, \dots, \alpha_d\}$$



Usage

In Python...

```
# polynomial basis
ef = ot.LinearEnumerateFunction(dim)
factC = [LegendreFactory()] * dim
prod = ot.OrthogonalProductPolynomialFactory(factC, ef)

# non-polynomial basis
factC = [ot.FourierSeriesFactory()] * dim
prod = ot.OrthogonalProductFunctionFactory(factC)

algo = ot.FunctionalChaosAlgorithm(...)
```

Rank one tensor

Rank one tensor

$$f(x_1, \dots, x_d) = \prod_{i=1}^d v_i(x_i)$$

with

$$v_i = \sum_{j=1}^{n_i} \alpha_j^{(i)} \phi_j(x_i)$$

expanding to

$$f(x_1, \dots, x_d) = (\alpha_1^{(1)} \phi_1(x_1) + \dots + \alpha_{n_1}^{(1)} \phi_{n_1}(x_1)) \times (\alpha_1^{(2)} \phi_2(x_2) + \dots + \alpha_{n_2}^{(2)} \phi_{n_2}(x_2)) \times \dots \times (\alpha_1^{(d)} \phi_1(x_d) + \dots + \alpha_{n_d}^{(d)} \phi_{n_d}(x_d))$$

Canonical tensor format

Available representation

$$f(x_1, \dots, x_d) = \sum_{k=1}^r \alpha_k \prod_{i=1}^d v_i^{(k)}(x_i)$$

with

$$v_{i} = \sum_{i=1}^{n_{j}^{(k)}} \alpha_{j}^{(i,k)} \phi_{j}(x_{i})$$



Alternating Least Squares

Alternating Least Squares algorithm

Allows to learn a rank-one tensor.

Algorithm 1 ALS

```
1: Initialize v_i(x_i) = 1
```

2: while v does not converge do

```
3: for i=1 to d \frac{do}{do}
```

$$\Psi^i(x)]_j = \prod_{u=1 \neq i}^d v_u(x_u) \phi_j^i(x_i)$$

5: Solve
$$\operatorname{argmin} ||y - \Psi^i(x)^t \beta_i||_2^2$$

6: end for

7: end while

Greedy rank-one approximation

Alternating Least Squares algorithm

Allows to learn a rank-r tensor.

Algorithm 2 Greedy rank-one

- Rank-1 approximation $\prod_{i=1}^{d} v_i^{(1)}(x_i)$
- 2: for r=2 to r_{max} do
- Rank-1 approximation $\prod_{i=1}^{d} v_i^{(r)}(x_i)$
- $y^m = y \sum_{k=1}^r \alpha_k \prod_{i=1}^{r-1} v_i^{(r)}(x_i)$ Update α to minimize error (least-squares)
- 6: end for



Usage

```
In Python...
r = 4 \# max rank
dim = 5
nk = [10] * dim
factC = [ot.FourierSeriesFactory()] * dim
prod = ot.OrthogonalProductFunctionFactory(factC)
X = dist.getSample(size)
Y = model(X)
algo = ot.TensorApproximationAlgorithm(X, Y, dist, factC, nk, r)
# L1 regularisation
lars = ot.LAR()
loo = ot.CorrectedLeaveOneOut()
aprox = ot.LeastSquaresMetaModelSelectionFactory(lars, loo)
algo.setApproximationAlgorithmFactory(aprox)
algo.run()
```

Conclusion

Conclusions

- Greedy rank-1
- Regularized greedy rank-one

Perspectives

Rank-k

