Correspondence Between Kriging with Inequality Constraints and Constrained Splines

Kriging and splines under constraints

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2. Inequality constraints (more challenging):
   - In practice, the true function may satisfy some inequality constraints over the whole domain with respect to some or all input variables.
   - The idea is to incorporate inequality constraints into a GP emulator.

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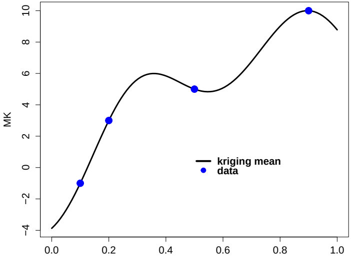

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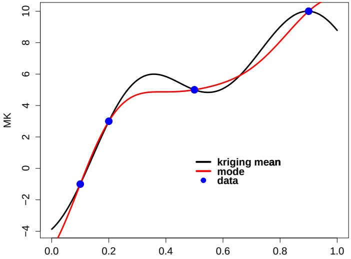

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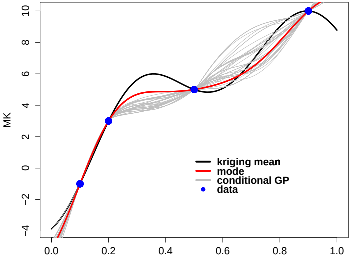

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Kriging with inequality constraints

- Let $\mathcal{C}$ be the subset of functions that satisfy the inequality constraints (e.g. the set of non-decreasing functions).
- Let $(Y(\mathbf{x}))_{\mathbf{x} \in [0,1]^d}$ be a centered GP with covariance function:

$$K(\mathbf{x}, \mathbf{x}') = cov(Y(\mathbf{x}), Y(\mathbf{x}')) = E(Y(\mathbf{x})Y(\mathbf{x}')).$$

- **Formulation of the general problem**: find the conditional distribution of the GP Y given observation data and inequality constraints

$$\begin{cases} Y(\mathbf{x}^{(i)}) = y_i, \quad i = 1, \ldots, n, \\ Y \in \mathcal{C}. \end{cases} \qquad (\mathcal{I} \cap \mathcal{C})$$

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Kriging with inequality constraints

- **Approximation method**: approximate the Gaussian process Y by a finite-dimensional Gaussian process Y^N

$$Y^N(x) = \sum_{j=0}^{N} \xi_j h_j(x), \qquad (1)$$

in which $\xi = (\xi_0 \ldots \xi_N)^\top$ is $\mathcal{N}(\mathbf{0}, \Gamma^N)$ and the basis functions h_j are deterministic.

Choice and property of the basis functions $(h_j)_{j=0,\ldots,N}$

The choice of the functions $\{h_j\}$ depends on the type of constraints and

- $Y^N(.)$ **in the strip** $[a, b]$ $\iff$ $a \leq \xi_j \leq b$; $j = 0, \ldots, N$.
- $Y^N(x)$ is **non-decreasing** $\iff$ $\xi_j \geq 0$; $j = 0, \ldots, N$.
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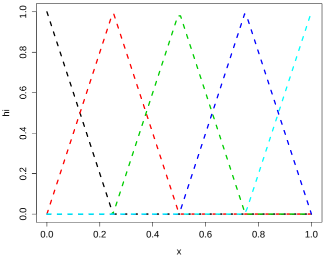
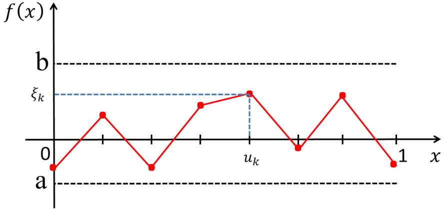
Bound constraints type basis functions

In this case, $\mathcal{C} = \{f \ : \ [0,1] \to \mathbb{R} \ : \ a \leq f(x) \leq b\}$.
Let $(u_k)_{k=0,\dots,N}$ be the subdivision such that $u_k = k/N$ and $(h_j)_j$ be the hat functions such that $h_j(u_k) = \delta_{j,k}$.





$f(x) = \sum_{j=0}^{N} \xi_j h_j(x)$ is the piecewise linear function with knots $(u_k)_k$ such that

$$f(u_j) = \xi_j, \qquad j = 0, \dots, N.$$

Thus, $\forall x, \ f(x) \in [a,b] \iff \forall j, \ \xi_j \in [a,b]$.

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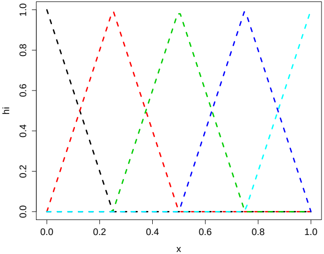

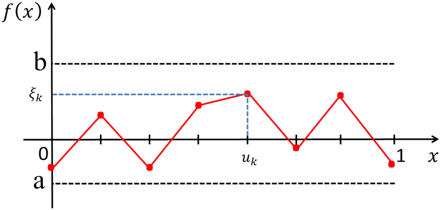

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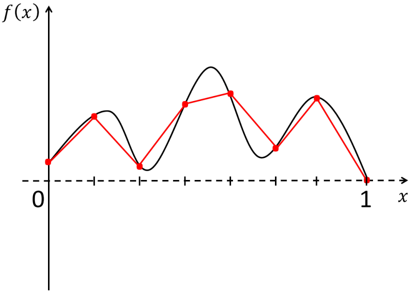
Covariance matrix of the coefficients

By the special choice of the basis functions, we have

$$Y^N(x) = \sum_{j=0}^{N} \xi_j h_j(x) = \sum_{j=0}^{N} Y^N(u_j) h_j(x).$$

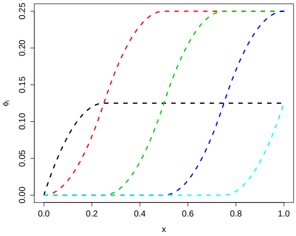
Hence, Y^N converges pathwise uniformly to Y if $Y^N(u_j) = Y(u_j)$ (with probability 1). So, we choose the covariance matrix Γ^N such that

$$\begin{aligned} \Gamma^N_{i,j} &= cov(\xi_i, \xi_j) \\ &= cov(Y(u_i), Y(u_j)) \\ &= K(u_i, u_j) \end{aligned}$$



Monotone basis functions $(\phi_j)_j$

We define ϕ_j $(j = 0, \ldots, N)$ such that $\phi_j(x) = \int_0^x h_j(t)dt$.



In this case, the approximation model is

$$Y^N(x) = \zeta + \sum_{j=0}^{N} \xi_j \phi_j(x) = Y(0) + \sum_{j=0}^{N} Y'(u_j)\phi_j(x). \qquad (2)$$

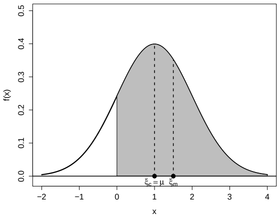
Thus, $\Gamma^N_{j,k} = cov(\xi_j, \xi_k) = cov(Y'(u_j), Y'(u_k)) = \frac{\partial^2 K(u_j, u_k)}{\partial x \partial x'}$.

New formulation of the problem

For monotonicity constraints, simulate the Gaussian vector ξ such that

$$\begin{cases} \sum_{j=0}^{N} \xi_j \phi_j(x_i) = y_i, \quad i = 1, \ldots, n & \text{(n interpolation linear equations)} \\ \xi_j \geq 0, \quad j = 0, \ldots, N & \text{(N+1 inequality constraints)} \end{cases} \quad (\tilde{\mathcal{I}} \cap \tilde{\mathcal{C}})$$

Hence, we need to simulate a truncated multivariate normal distribution.



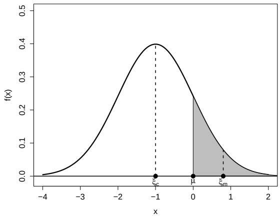


Figure: The mean is inside (resp. outside) the acceptance region (resp. right figure).

Definition

We denote $\xi_m = E\left(\xi \middle| \xi \in \tilde{\mathcal{I}} \cap \tilde{\mathcal{C}}\right)$. Then, the constrained kriging mean is equal to

$$m_{KI}^N(x) := E\left(\sum_{j=0}^{N} \xi_j \phi_j(x) \middle| Y^N(x_i) = y_i,\ \xi \in \tilde{\mathcal{C}}\right) = \sum_{j=0}^{N} (\xi_m)_j \phi_j(x) \qquad (3)$$

Let μ be the mode of the truncated Gaussian vector ξ. Then

$$\mu = \arg \min_{\boldsymbol{c} \in \tilde{\mathcal{I}} \cap \tilde{\mathcal{C}}} \left(\frac{1}{2} \boldsymbol{c}^\top \left(\Gamma^N\right)^{-1} \boldsymbol{c}\right), \qquad (4)$$

where Γ^N is the covariance matrix of the Gaussian vector ξ.

Definition

The function mode (Maximum A Posteriori) is defined as

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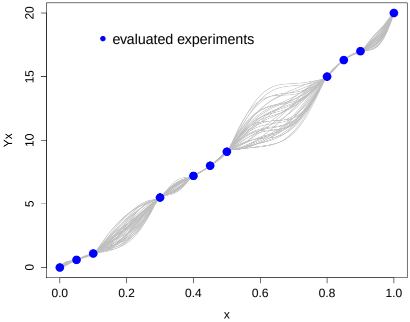

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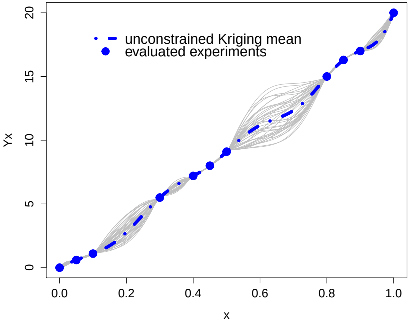

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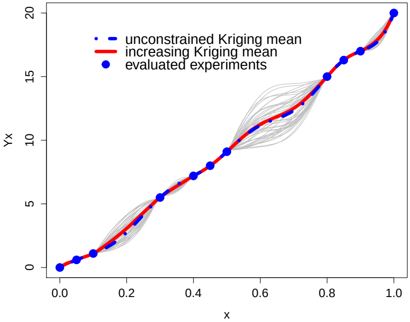

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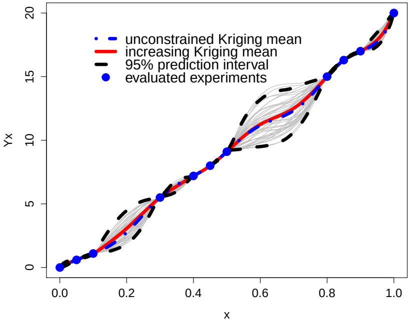

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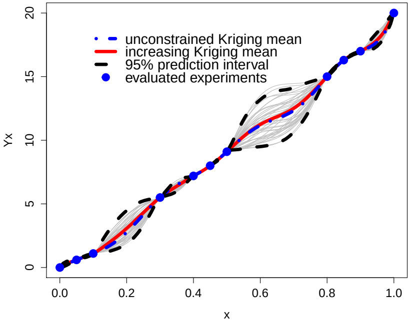


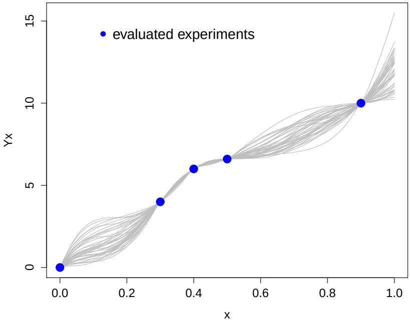
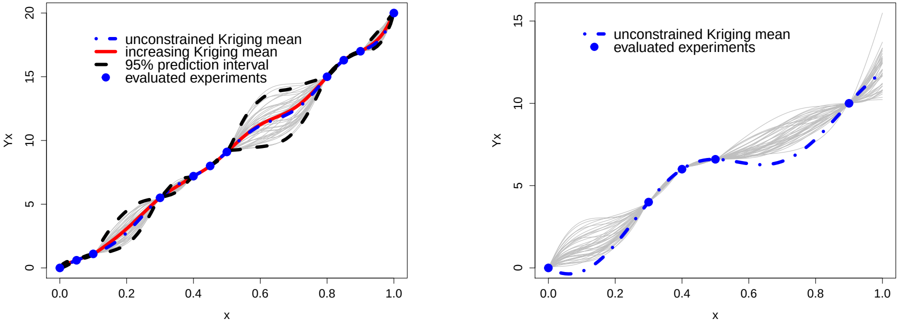


Figure: Simulated paths (gray lines) drawn from the conditional Gaussian process. The usual Kriging mean (blue dash-dotted line) coincides with the mode and respects monotonicity in left figure, but not in right figure. The red line defined as the mean of the simulated paths respects the monotonicity constraint everywhere.

Illustration for monotonicity constraint



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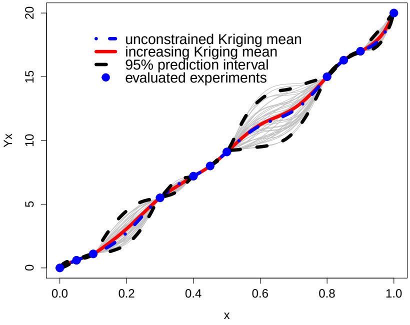

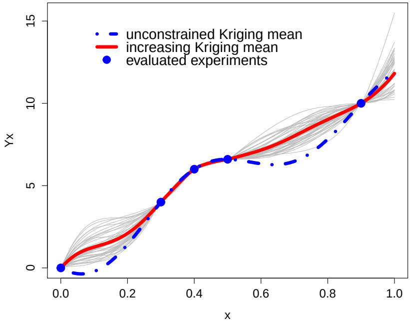

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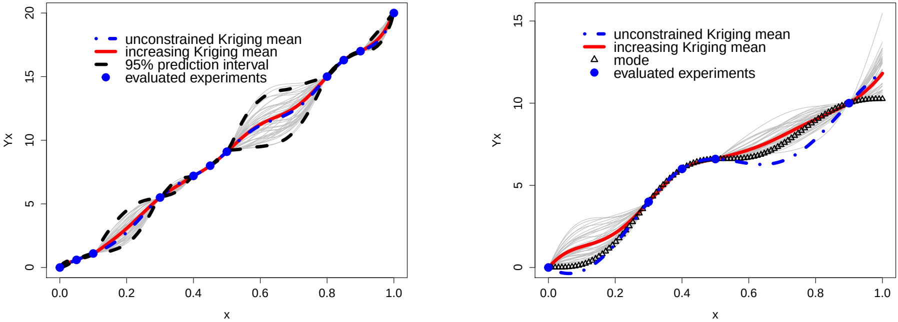

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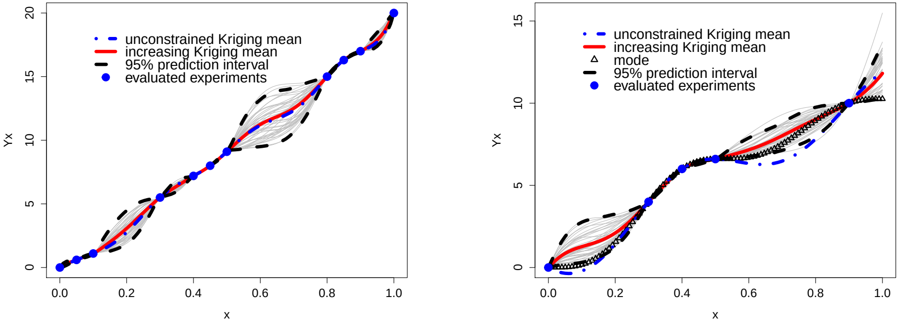

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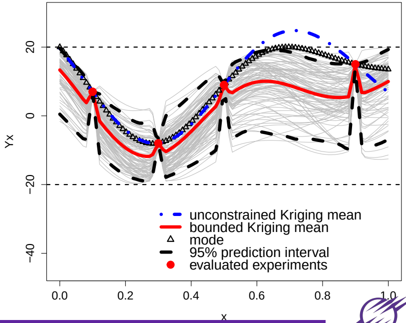
Illustration for bound constraint

For bound type constraint, the approximation model is

$$Y^N(x) = \sum_{j=0}^{N} \xi_j h_j(x) = \sum_{j=0}^{N} Y(u_j) h_j(x). \quad (5)$$

- The basis functions $h_j,\ j = 0, \ldots, N$ are the hat functions.
- The simulated paths drawn from the conditional GP are lying between $a = -20$ and $b = 20$ everywhere.
- Mode estimator respects both equality conditions and inequality constraints and is seen to be smooth.



Monotonicity in the 2-dimensional case

The input $x = (x_1, x_2)$ is supposed in $[0,1]^2$. We define monotonicity of f with respect to the two input variables as

$$\forall x_1 \in [0,1],\ x_2 \longmapsto f(x_1, x_2) \textit{ is } \text{non-decreasing}$$

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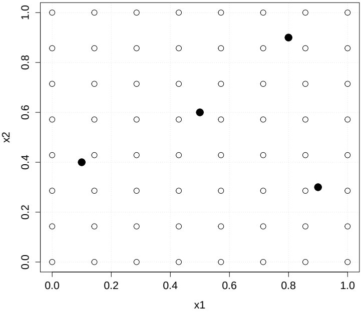


Monotonicity in the 2-dimensional case

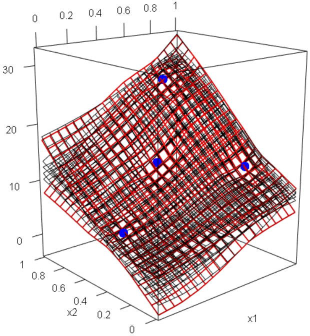
For 2D-monotonicity, the approximation model is:

$$Y^N(x_1, x_2) = \sum_{i,j=0}^{N} Y^N(u_i, u_j) h_i(x_1) h_j(x_2) = \sum_{i,j=0}^{N} Y(u_i, u_j) h_i(x_1) h_j(x_2), \qquad (6)$$

where $h_j,\ j = 0, \ldots, N$ are the 1D - hat functions (associated to knots $(u_j)_j$).

Y^N is monotone with respect to x_1 and x_2 iff

- $Y(u_{i-1}, u_j) \leq Y(u_i, u_j)$
  $Y(u_i, u_{j-1}) \leq Y(u_i, u_j),$
  $i, j = 1, \ldots, N.$
- $Y(u_{i-1}, u_0) \leq Y(u_i, u_0), \quad i = 1, \ldots, N.$
- $Y(u_0, u_{j-1}) \leq Y(u_0, u_j), \quad j = 1, \ldots, N.$



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Correspondence with optimal smoothing splines

We consider the following optimization problem :

$$\inf_{h \in H \cap I \cap C} \|h\|_H^2, \qquad (P)$$

where H is a RKHS with reproducing kernel K, I is the space of interpolation conditions and C is a convex set.

Theorem (Kimeldorf and Wahba 1970)

The problem (P) with no inequality constraint has a unique solution given by

$$h_{opt}(x) = \boldsymbol{k}(x)^\top \mathbb{K}^{-1} \boldsymbol{y}, \qquad (7)$$

where $\boldsymbol{y} = (y_1, \ldots, y_n)$, $\boldsymbol{k}(x) = (K(x_i, x))_{i=1,\ldots,n}$ and $\mathbb{K} = (K(x_i, x_j))_{i,j=1,\ldots,n}$.

Proof.

See Kimeldorf and Wahba 1970. □

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Correspondence with optimal smoothing splines

Theorem (X.Bay, L.Grammont and H. Maatouk, 2015)

The mode estimator (Maximum A Posteriori)

$$M_{KI}^{N} = \sum_{j=0}^{N} \mu_j \phi_j(x)$$

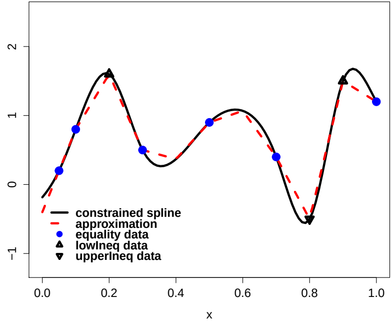
is (uniformly) convergent with N and the limit estimator ($N = +\infty$) is the constrained interpolation spline h_{opt}, solution of the previous problem (P):

$$h_{opt} = \arg \min_{h \in H \cap I \cap C} \|h\|_H^2$$

Proof.

See Bay et al. (2015). □

Constrained splines with finite number of inequality constraints



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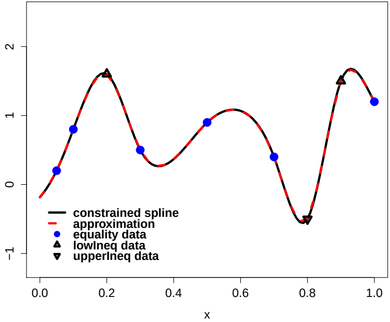

Constrained splines with finite number of inequality constraints

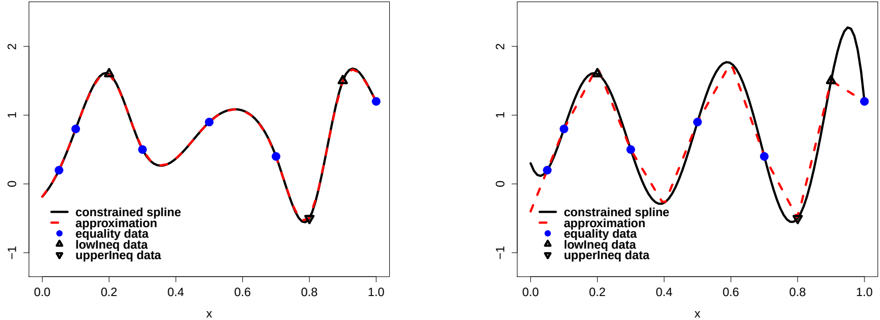

Figure: The black line represents the constrained interpolation spline using the Matérn 3/2 covariance function (left figure) and the Gaussian covariance function (right figure). The red dashed line correspond to the mode of the conditional GP for $N = 10$ and $N = 40$.

Constrained splines with finite number of inequality constraints

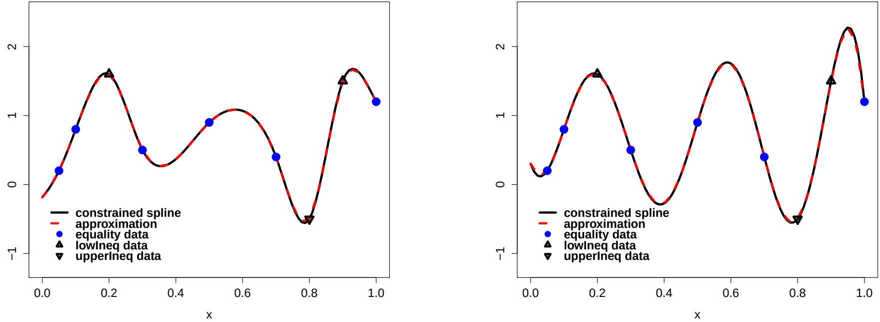

Figure: The black line represents the constrained interpolation spline using the Matérn 3/2 covariance function (left figure) and the Gaussian covariance function (right figure). The red dashed line correspond to the mode of the conditional GP for $N = 10$ and $N = 40$.

Constrained Cubic Spline Interpolation

- Cubic splines can be defined as functions minimizing the following well-known criterion (linearized energy (LE) measure, see e.g. Wolberg and Alfy (2002)):

$$E_L = \int_0^1 \left(f''(t)\right)^2 dt, \tag{8}$$

given the n observations (interpolation conditions) $f(x_i) = y_i$, $i = 1, \ldots, n$.

- With additional inequality constraints (such as bound, monotonicity or convexity constraints), the function minimizing the LE criterion is called a constrained cubic spline.

Monotone Cubic Spline Interpolation FC's Data

Table: RPN 15A Fritsch and Carlson (1980) data (LLL radiochemical calculations).

x	$f(x)$
7.99	0
8.09	2.76429e-5
8.19	4.37498e-2
8.7	0.169183
9.2	0.469428
10	0.943740
12	0.998636
15	0.999919
20	0.999994

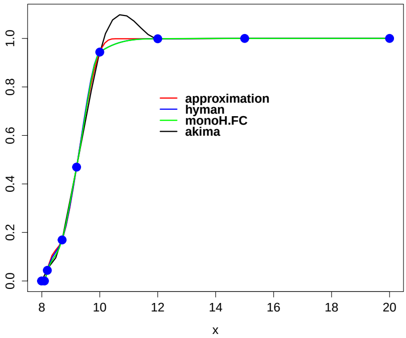

Figure: The monotone cubic spline interpolation for four different methods: Hyman's spline, FC's spline, Akima's spline and our approach.

Monotone Cubic Spline Interpolation FC's Data

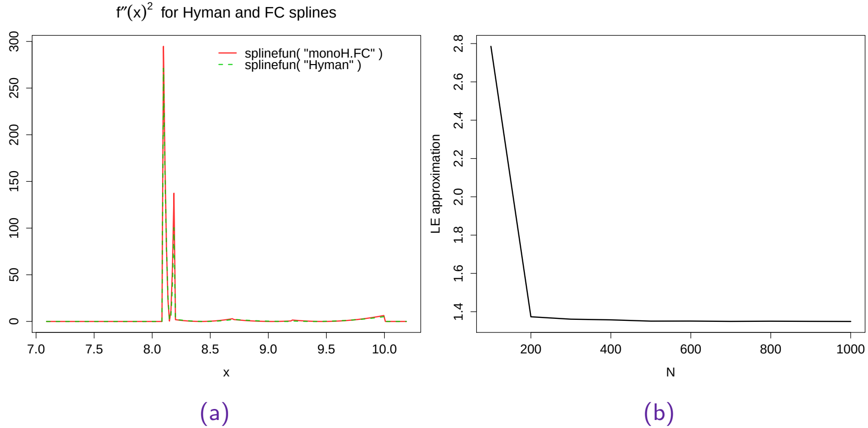

Figure: Approximate LE criterion for our algorithm using FC's data (Figure 5b). Comparison between "Hyman" and "FC" splines (Figure 5a). Notice that the LE criterion for Hyman's spline is slightly smaller and it is equal to 9.35.

Monotone Cubic Spline Interpolation using Wolberg's Data

Table: Wolberg and Alfy (2002) data used to compare different methods.

x	$f(x)$
0.0	0.0
1.0	1.0
2.0	4.8
3.0	6.0
4.0	8.0
5.0	13.0
6.0	14.0
7.0	15.5
8.0	18.0
9.0	19.0
10.0	23.0
11.0	24.1

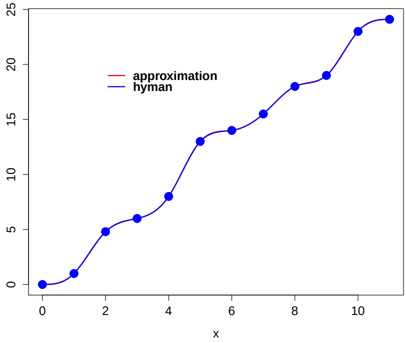

Figure: Monotone cubic splines using Wolberg's data: Hyman's method (blue line) and approximation $\hat{h}_N$ with $N = 1000$ (red line).

Monotone Cubic Spline Interpolation using Wolberg's Data

Table: Linearized energy measure using Worlberg's data.

Method	E_L
our approximation	**131.68**
Hyman	133.19
CSE	132.91
FE	**131.68**
LE	**131.68**
SDDE	223.55
MDE	131.71
FB	236.30

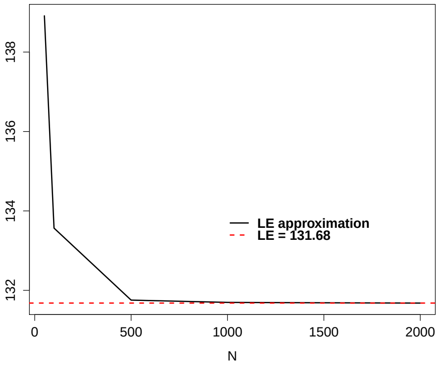

Figure: Approximate LE measure for our algorithm using Wolberg's data.

Real application in finance to estimate the term structure of interest rates

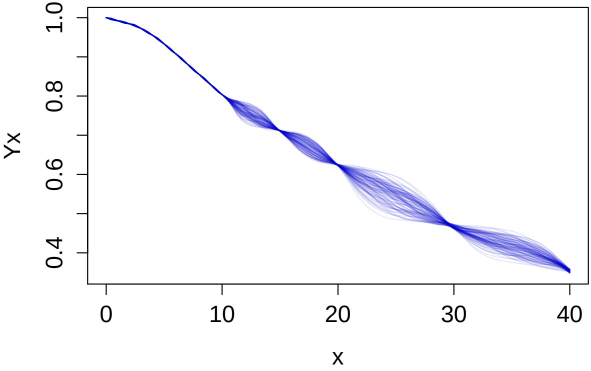

Figure: Simulations paths drawn from the conditional Gaussian process with monotonicity constraints using real data to estimate the interest rate.

Outline

Conclusion and future work

Conclusion

- We propose a new approximation method for incorporating both equality conditions and inequality constraints into a GP emulator. The inequality constraints are satisfied everywhere.
- The simulation of the conditional GP is equivalent to generate a Truncated Gaussian Vector (restricted to a convex set).
- The mode (Maximum A Posteriori) of the finite-dimensional conditional GP converges uniformly to the constrained interpolation spline.
- Comparison with existing monotone cubic spline algorithms in terms of linear energy criterion is shown.

Future work

- Convergence of the mode estimator to the constrained interpolation spline using smooth basis functions.
- Choice of the knots (subdivision of the input set).

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Thank you for your attention.