Non-parametric regression using splines, with applications

Lecture dedicated to the memory of Milcho Tsvetkov

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ACKNOWLEDGEMENTS

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Based on joint research with H. Render, Ts. Tsachev.

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- V. A. Baturin, W. Däppen, A. V. Oreshina, S. V. Ayukov and A. B. Gorshkov, **Interpolation of equation-of-state data**, A&A, Volume 626, June 2019.

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- Collin A. Politsch, Jessi Cisewski-Kehe, Rupert A. C. Croft, and Larry Wasserman, **Trend Filtering – I. A Modern Statistical Tool for Time-Domain Astronomy and Astronomical Spectroscopy**, 2020

A special non-parametric model - Cubic splines S(x) - a reminder

- $S(x)$ is a piecewise cubic polynomial in every interval (x_i, x_{i+1}), where $a = x_1$ and $b = x_n$, and the **knots** x_j satisfy

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- **THEOREM**. For every set of interpolation data $\{f_i\}_{i=1}^n$ defined at $\{x_i\}_{i=1}^n$ there exists a unique (Natural) spline $S(x)$ with breaks at $\{x_i\}$ s.t.

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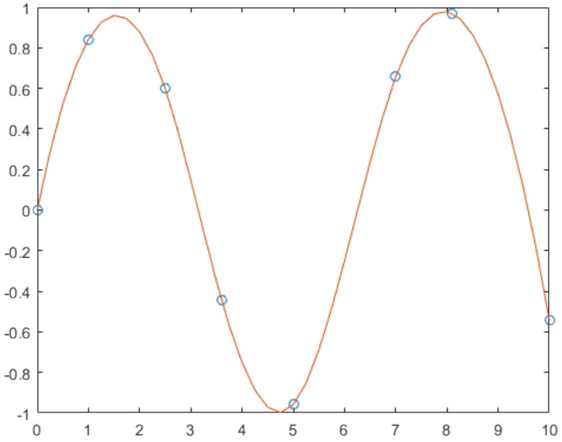
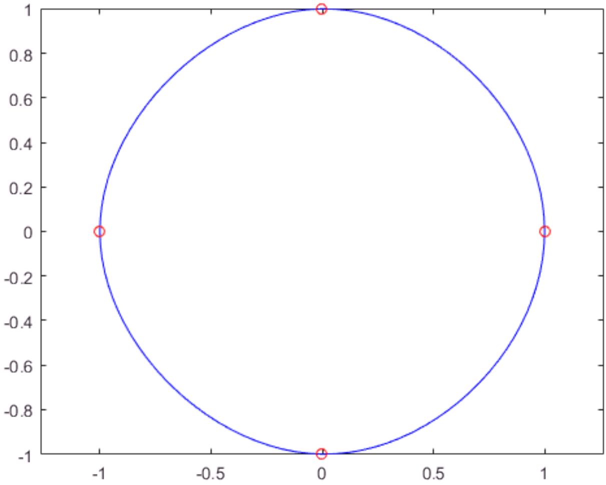
- References: Sommerfeld (1903), de Boor (1978, 2001), Stoer-Bulirsch (1998), Green-Silverman (1994).

Why are polynomial splines good? An example - the sin function



Example - the circle



Fast algorithms for computation of interpolation cubic splines

- Fast algorithms exist for large amount of data (cf. **Wahba** 1990, **Green-Silverman** 1994)

- Assume data values $\mathbf{Y} = \{Y_j\}$ measured at $x_j \in [a, b]$, for $j = 1, ..., N$

The Smoothing cubic spline - Finding trends

- Assume data values $\mathbf{Y} = \{Y_j\}$ measured at $x_j \in [a, b]$, for $j = 1, ..., N$
- We consider the penalized functional

$$S(g) = \sum_{j=1}^{N} (g(x_j) - Y_j)^2 + \lambda \int_a^b |g''(t)|^2 \, dt$$

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- **THEOREM**. The solution to problem

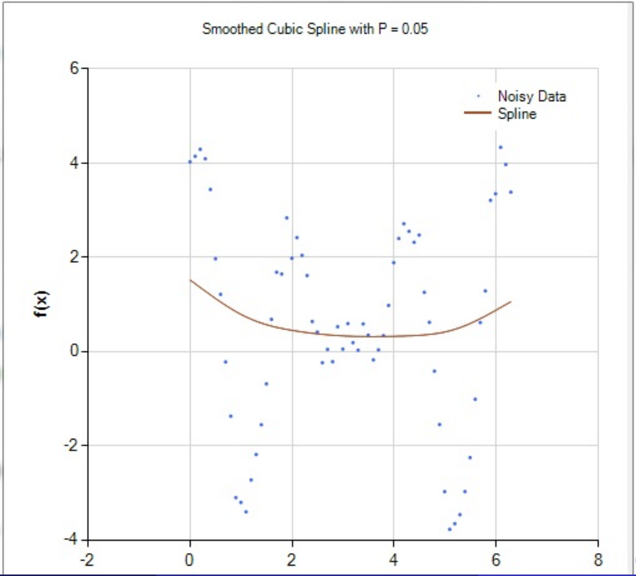
$$\min_g S(g) \qquad \text{where } g \in C^2(a, b)$$

is a cubic spline, with knots $\{x_j\}$ and interpolation data

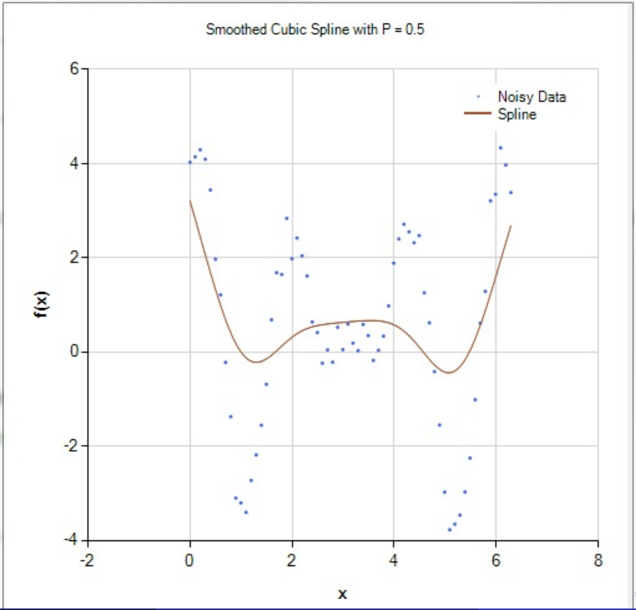
$$\mathbf{g} = (I + \lambda K)^{-1} \mathbf{Y}$$

where $K = QR^{-1}Q^T$.

Examples of smoothing splines with different lambda; here lambda = 0.95

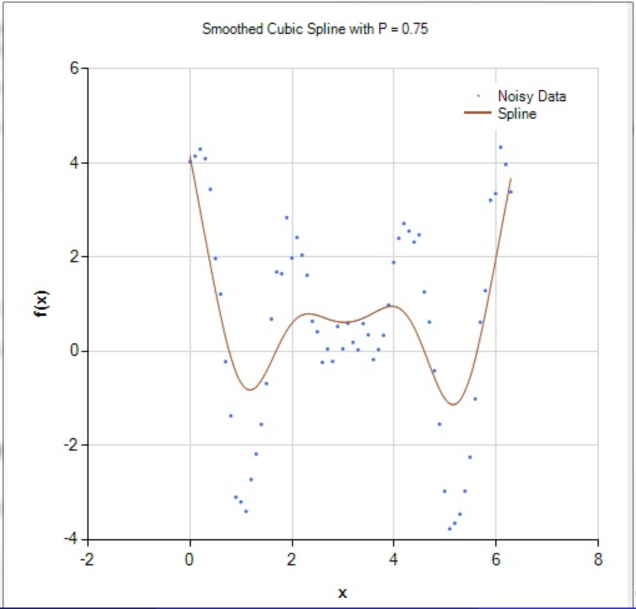


lambda is 0.5

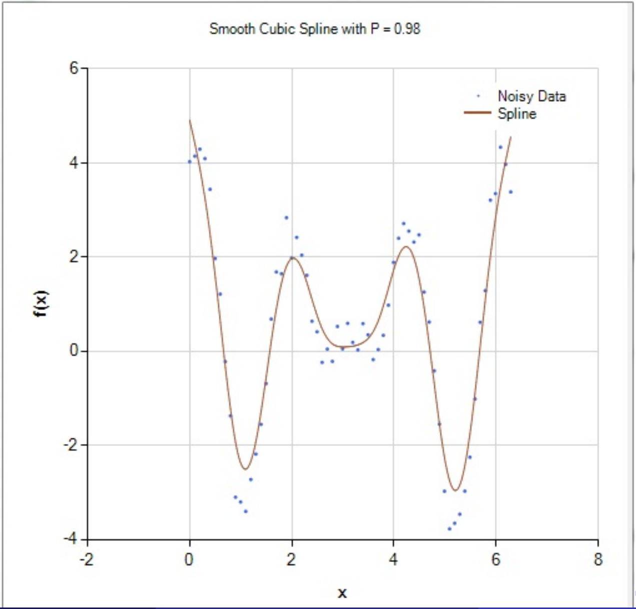


Smoothed Cubic Spline with P = 0.5
Noisy Data
Spline
f(x)
x
6
4
2
0
-2
-4
-2
0
2
4
6
8

lambda is 0.25 - more wiggling



lambda is 0.02 - very wiggling



The fast (O(n) time) Reinsch algorithm (1971)

FACT: There exists a fast algorithm of Reinsch for the computation of the smoothing splines. Reference: Stoer-Bulirsch, Numerical Analysis, Springer, 2010.

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- The cross-validation (leave-one-out) score function is

$$CV(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \left(Y_i - \widehat{g}^{(-i)}(t_i;\lambda) \right)^2$$

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- We **minimize** $CV(\lambda)$ to find λ.

The representation of Cross-Validation and GCV

- **THEOREM**: We have

$$CV(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{Y_i - \widehat{g}(t_i; \lambda)}{1 - A_{ii}(\lambda)} \right)^2$$

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$$A(\lambda) = \left(I + \lambda Q R^{-1} Q^T\right)^{-1}$$

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- Similar formula for Generalized Cross Validation - see the same references

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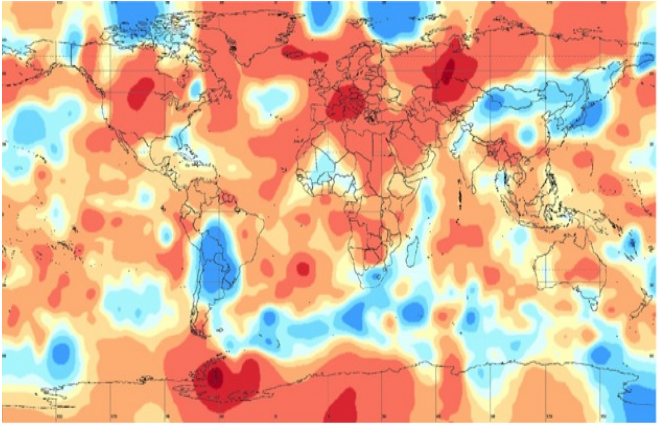
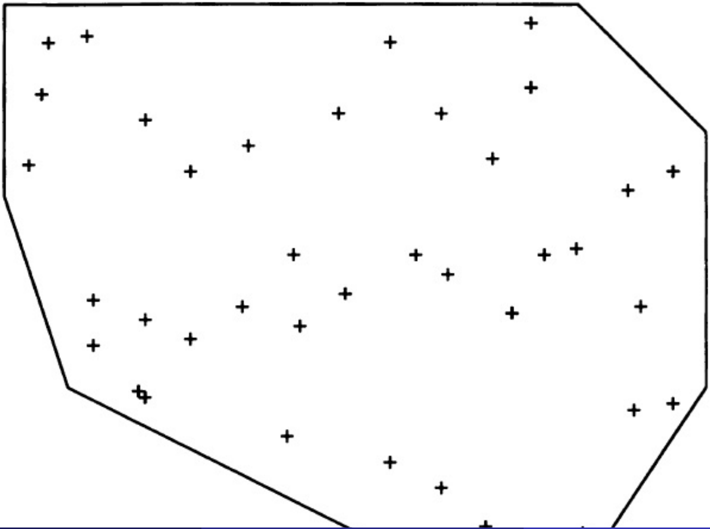
- One may use also RBFs, Kriging, Minimum Curvature, Shepard's method, etc. And our approach - POLYSPLINES.

Smoothed data - an example



Example of Multidimensional Scattered data set

- Importance for life problems even in dimension 2 – data of Earth Observations,



The generalized L-splines - the main bricks of the Polysplines

- Instead of 1D polynomials we use piecewise exponential functions called $L-$splines. A special case: fix ξ, then the $L-$spline is defined as a piecewise solution in every interval $[x_j, x_{j+1}]$ of the equation:

$$L_\xi f(t) = 0 \qquad \text{with } L_\xi = \left(\frac{\partial^2}{\partial t^2} - \xi^2\right)^2$$

which is C^2 at the knots x_j; the basis of solutions are $e^{t\xi}, te^{t\xi}, e^{-t\xi}, te^{-t\xi}$, while for the classical case are $1, t, t^2, t^3$.

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- A much bigger generalization: Consider a polynomial L of degree 4 and the solutions of the related differential operator

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- In the case of real coefficients of the polynomial L with four different roots a_j the basis of all solutions is given by the exponential functions $e^{a_j t}$.

Examples of L-splines

- Interpolation and smoothing $L-$splines of the special form depending on ξ were considered exhaustively, with fast algorithms in a paper **"On a class of L-splines of order 4: fast algorithms for interpolation and smoothing"**, BIT Numerical Mathematics, 2020. They have as basis the exponential functions $e^{\xi t}, te^{\xi t}, e^{-\xi t}, te^{-\xi t}$.

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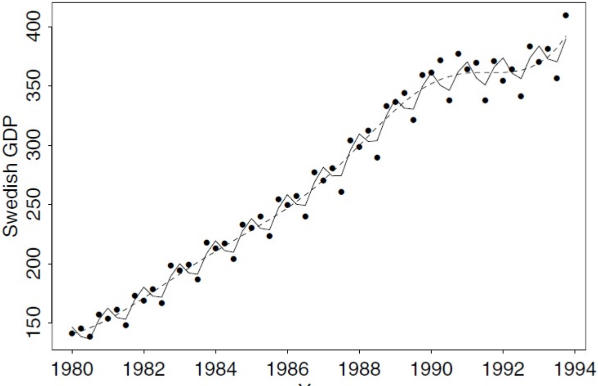
- These 1D $L-$splines are **important for the multidimensional theory of polysplines**.
- The case of more general $L-$splines of order 4 is considered in a more recent paper **"Fast algorithms for interpolation with L-splines for differential operators L of order 4 with constant coefficients"** , in ARXIV, submitted in J. Comp. and Applied Maths.

Further motivating examples to study smoothing L-splines (and exponential splines)

- GDP for Sweden with seasonal variation (in Ramsay-Silverman, 2005) – a cyclic effect superimposed on a linear development



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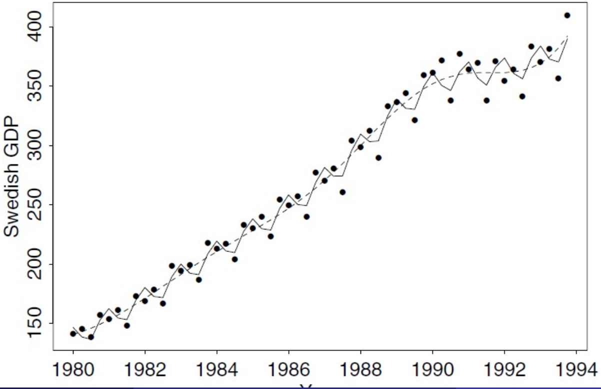
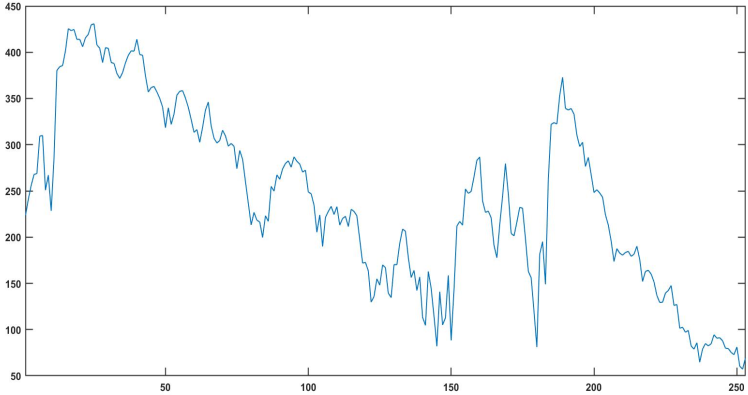
- the dashed line is Cubic smoothing (with GCV for λ), and the solid line is a smoothing $L-$spline with $L = \left(-\gamma \frac{d}{dt} + \frac{d^2}{dt^2}\right)\left(\omega^2 + \frac{d^2}{dt^2}\right)$.



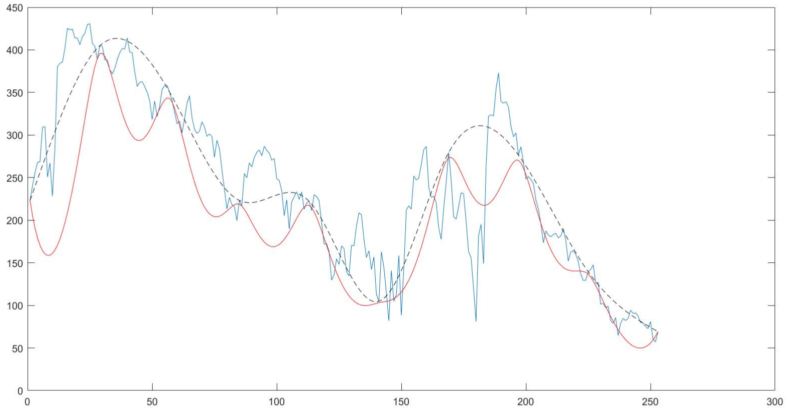
Examples of smoothing L-splines - S&P 500 data

- Daily S&P500 prices for the period 24 October, 2017 – 24 October, 2018, total 253 days.



Smoothing results for the operator L_xi

- for $N = 10$ knots; $\lambda = 3$, $\xi = 0.01$ (dash) and $\xi = 0,13$:



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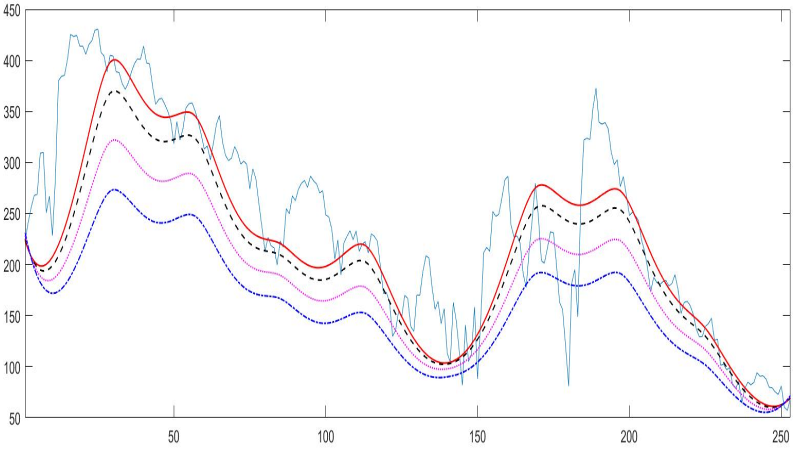
- for $N = 10$ knots; $\lambda = 5, 30, 80, 150,$ and $\xi = 0.13$.



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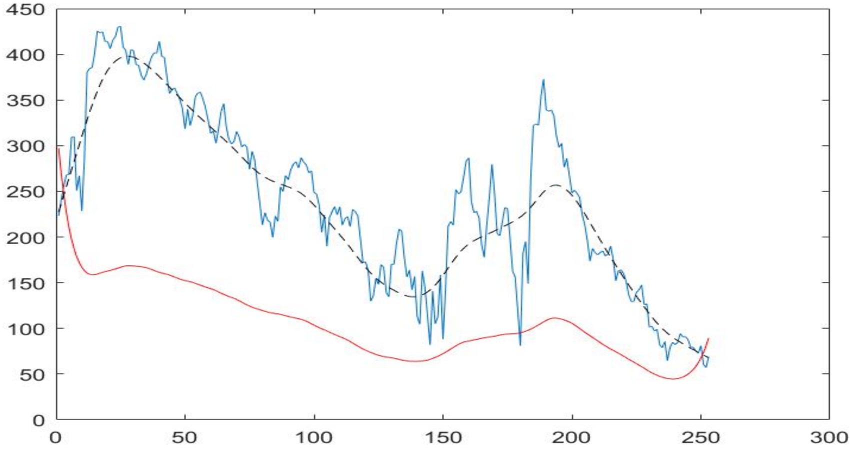
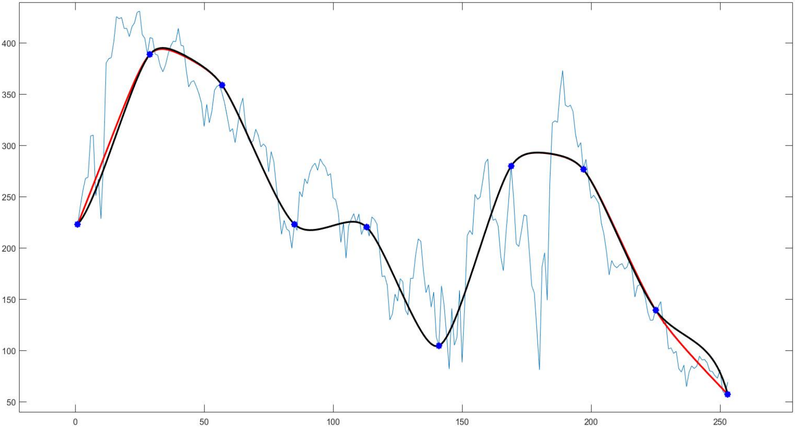
- for $N = 30$ knots; $\lambda = 500$, and $\xi = 0.01$ and $\xi = 0.13$:



The new $L-$splines on the S&P500 data



The new $L-$splines - some subtleties

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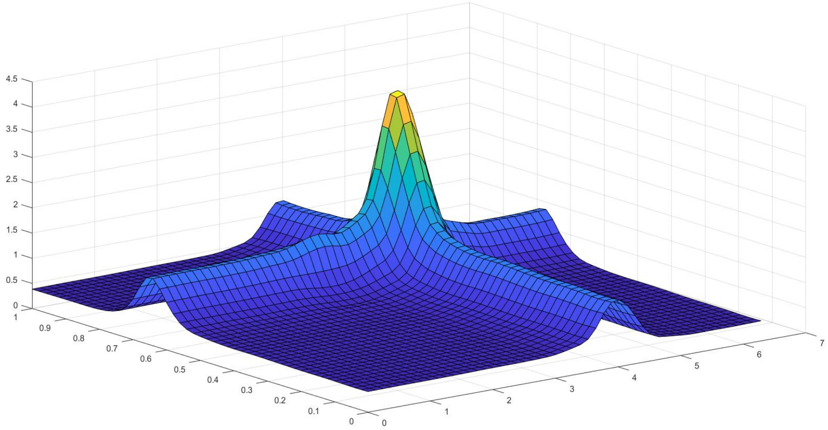
Polyspline interpolating 2D Titanium data at 70 points



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- THANK YOU !