Gaussian process regression fast solver

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Outline

Introduction

In numerical analysis, interpolation is an employed method of fitting a function by constructing new data points within the range of some discrete known set of points. So we basically use sampled points to estimate values at other unknown points.

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There are numerous interpolation techniques, such as inverse distance method, natural neighbour, polynomial regression, splines and Gaussian process regression.

Gaussian regression

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The model, majorly consist of two components, given by

$$y(x) = \mu + \epsilon(x)$$

where μ is the large scale variation and $\epsilon(x)$ the small scale spatial autocorrelation.

Gaussian regression

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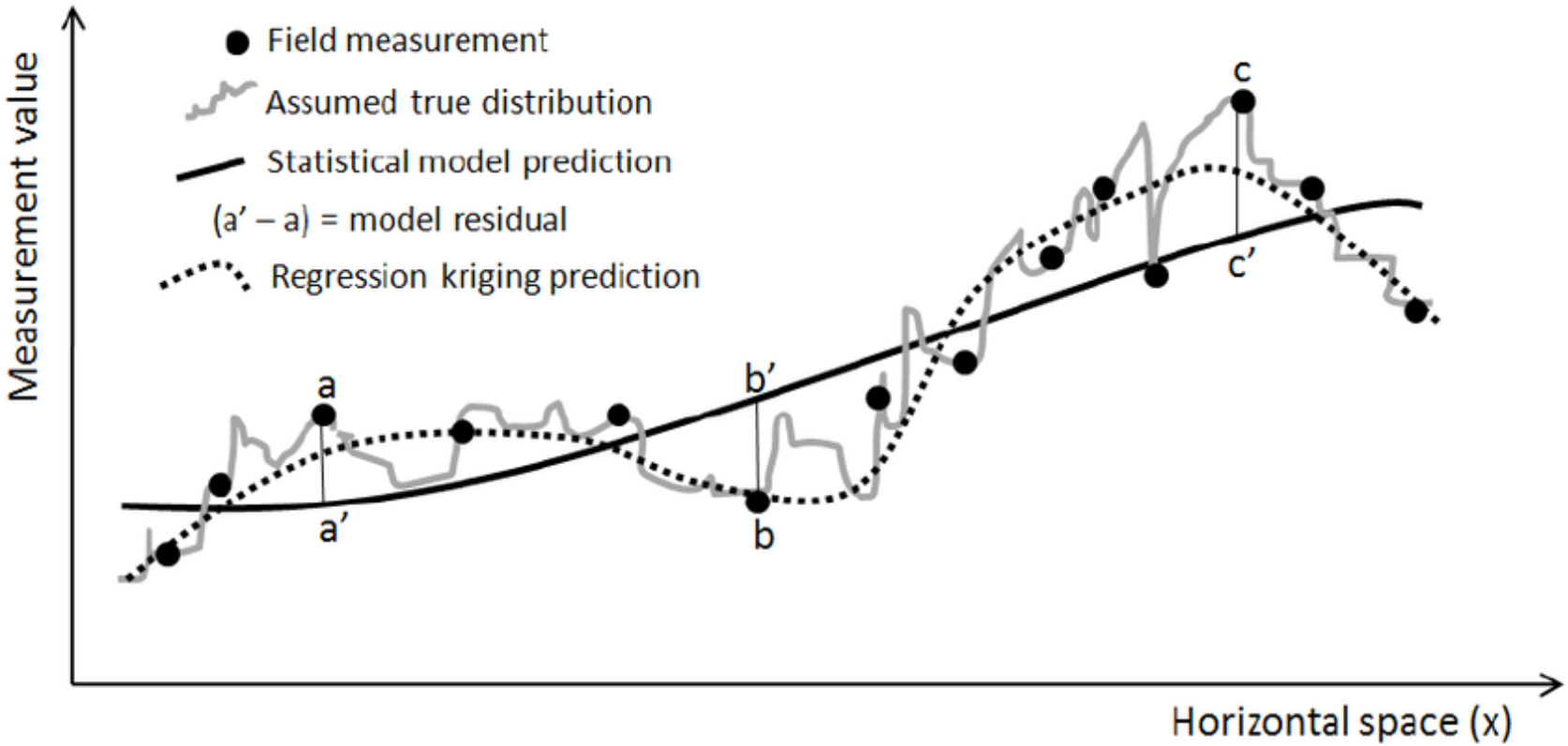

Рис.: Kriging Vs OLS interpolation
https://www.researchgate.net/figure/265075728_fig4

Model specification

Let x be a vector of sampled locations, y a vector of function values, z a vector of locations where we are interested in function value. Then, to find the function values y' at the points z, we do the following:

$$y' = \mu + K_{zx} K_{xx}^{-1}(y - \mu \mathbf{e}),$$

$(K_{xx})_{ij} = \exp(-\theta|x_i - x_j|^p)$, covariance of observed location

$(K_{zx})_{ij}$ covariance between the new locations and observed locations.

The parameters θ and p are estimated e.g. by method of maximum likelihood

Project goals

- Implement fast kriging on Python and test it on geodata

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- Implement fast kriging on Python and test it on geodata
- Write a plugin for QGIS realizing this solution

Fast kriging for evenly spaced grids

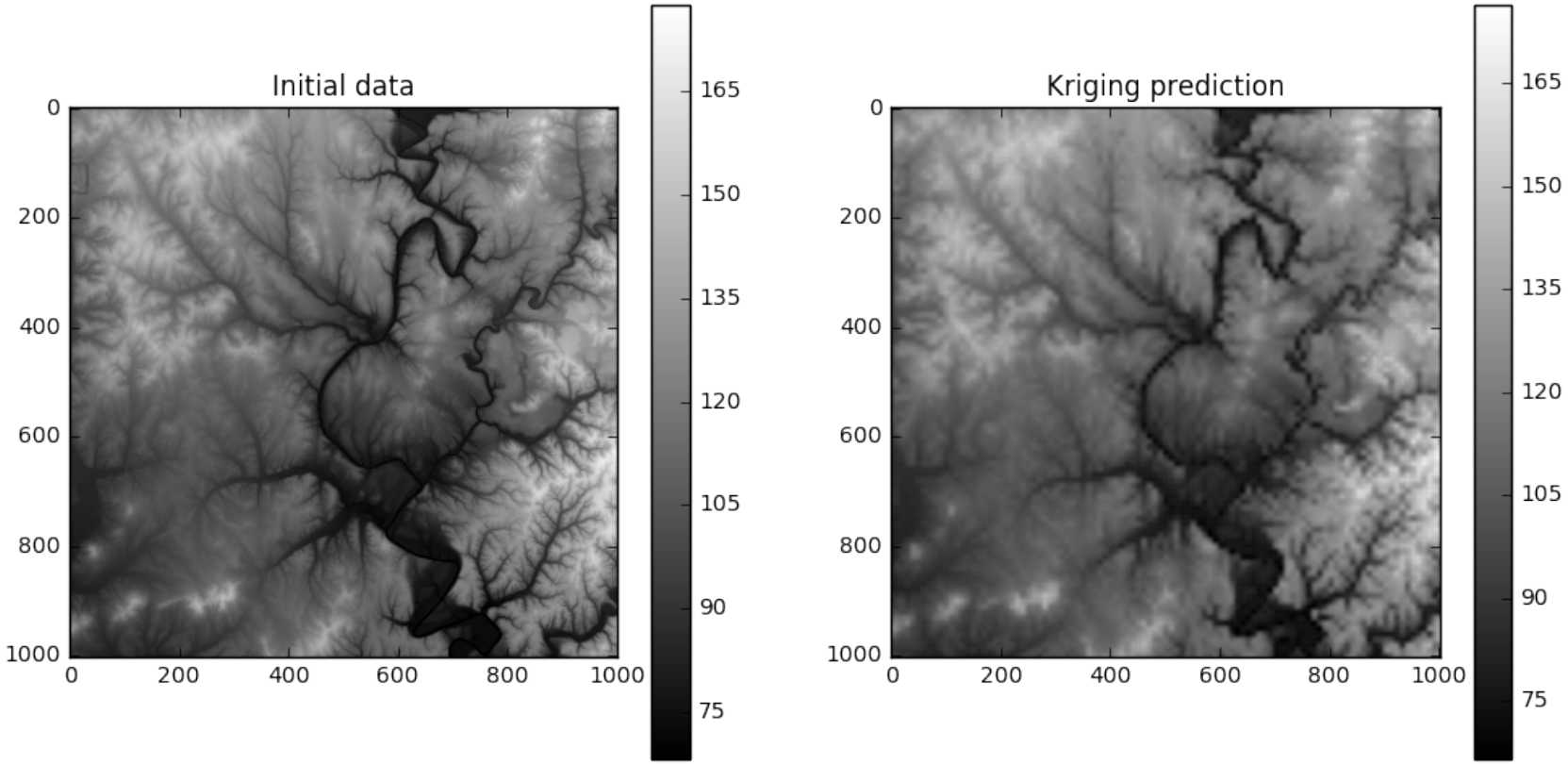
The structure of K_{xx} depends on selection of data points
Evenly spaced points yield a Toeplitz matrix (or BTTB for 2D):

$$(K_{xx})_{ij} = \exp(-\theta|x_i - x_j|^p) = (K_{xx})_{i+q,j+q}.$$

This allows us to perform fast matrix-vector product and thus solve linear systems faster

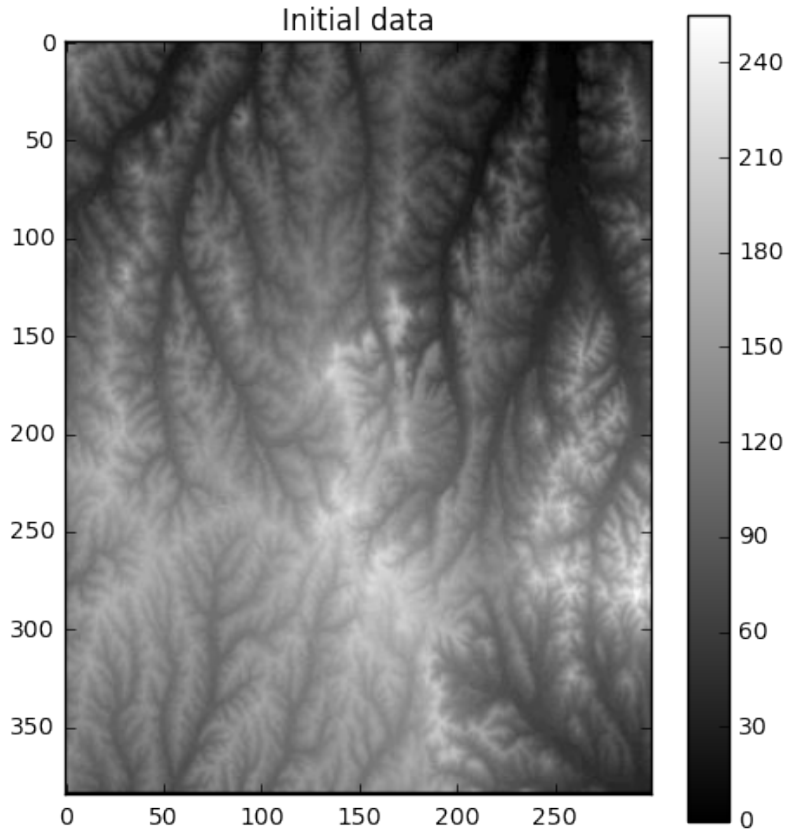
Results

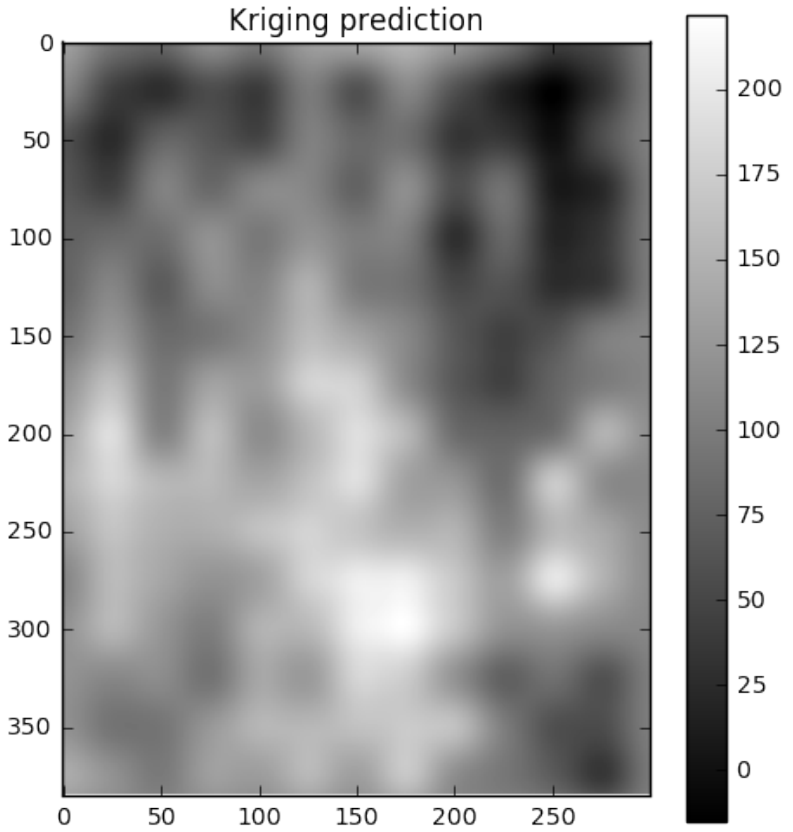
Prediction here is based on 100x100 points. For this test sample, $\|y' - y_{true}\|_2 / \|y_{true}\|_2 = 0.026$; $\sqrt{\sigma^2}/\mu = 0.132$



Results

Prediction here is based on 12x16 points. For this test sample, $\|y' - y_{true}\|_2 / \|y_{true}\|_2 = 0.193$; $\sqrt{\sigma^2}/\mu = 0.334$

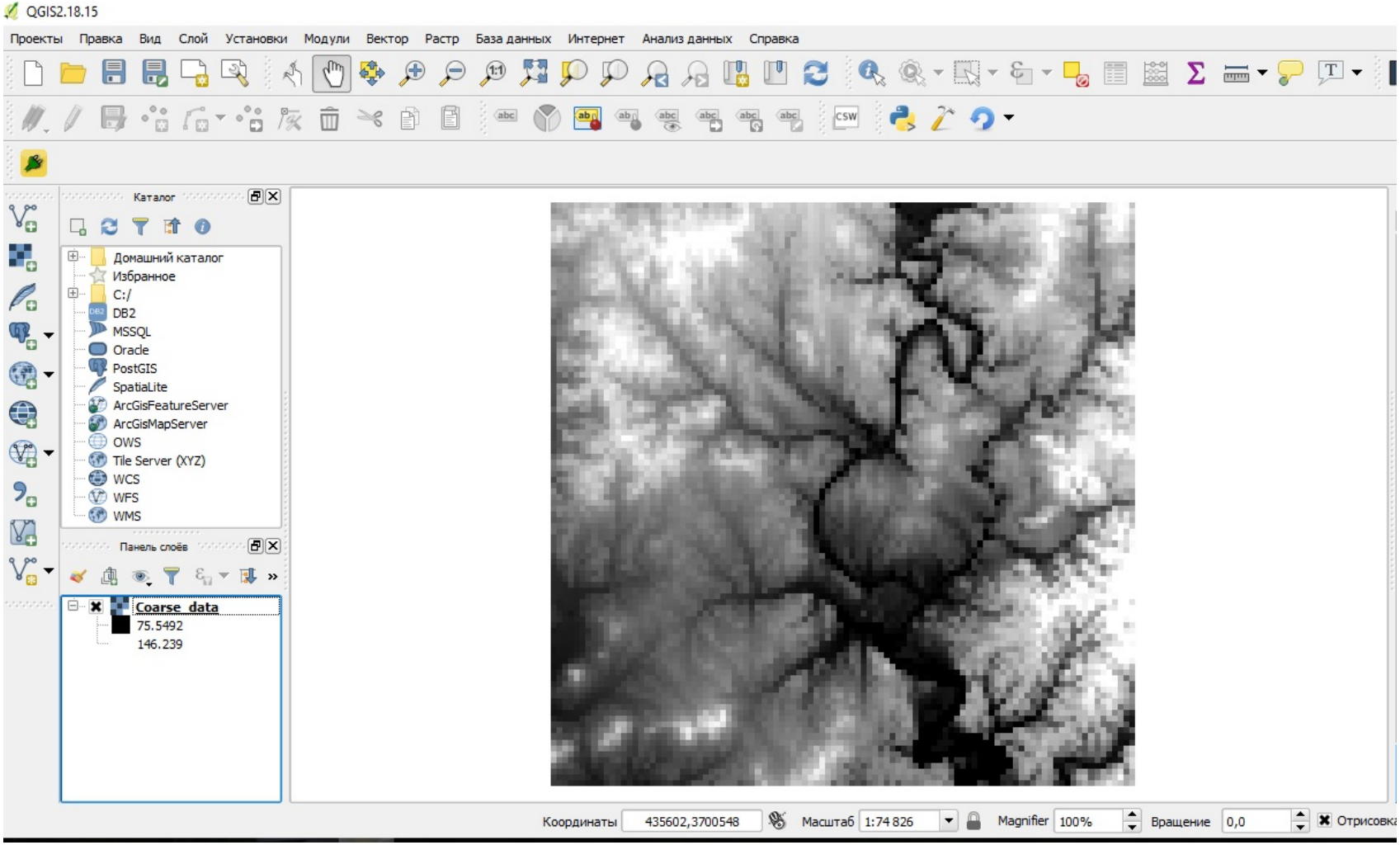




QGIS

QGIS is a free and open-source cross-platform desktop geographic information system application.
Its modular structure enables creation of plugins.
To our knowledge, existing kriging solutions don't take advantage of matrix structure

QGIS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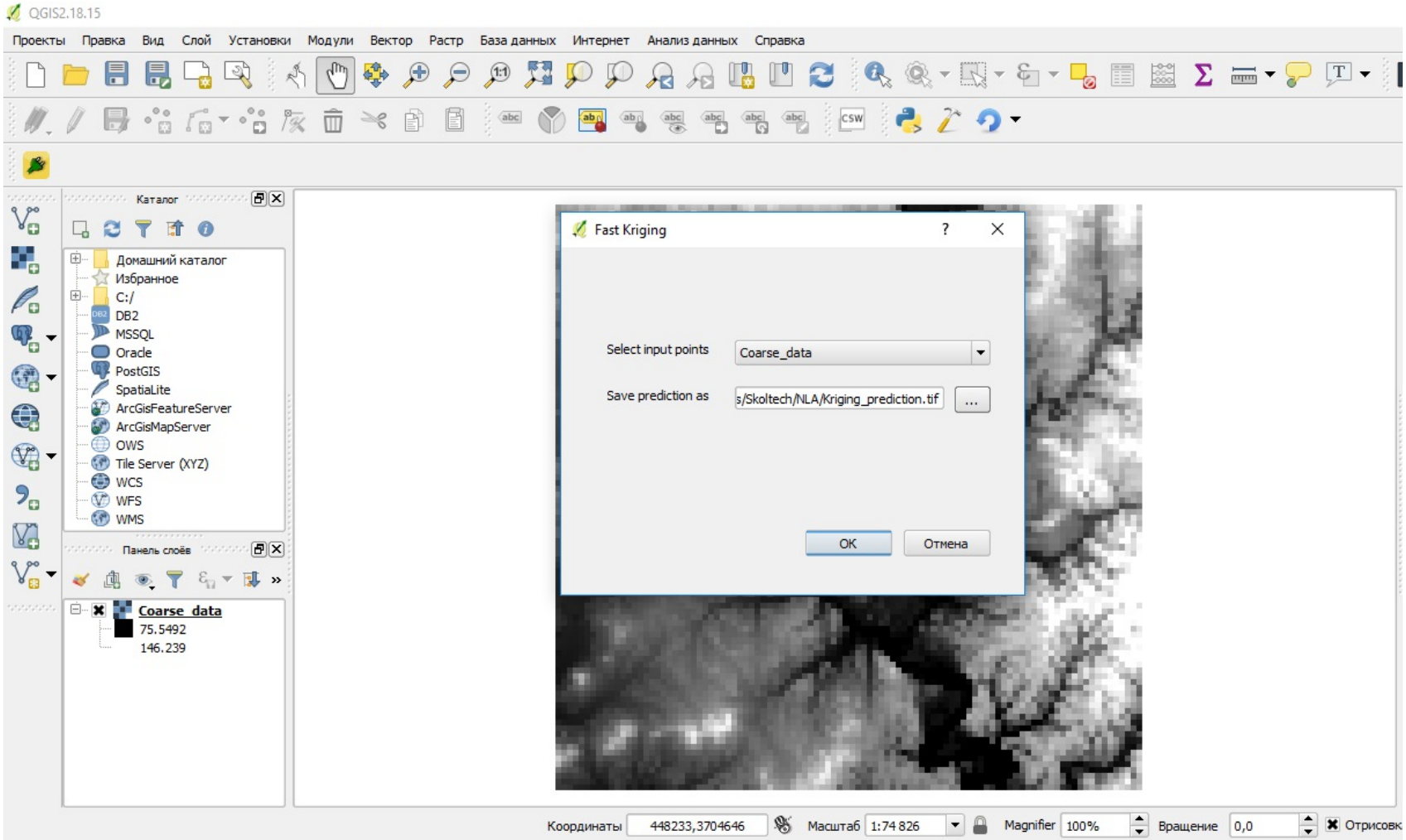
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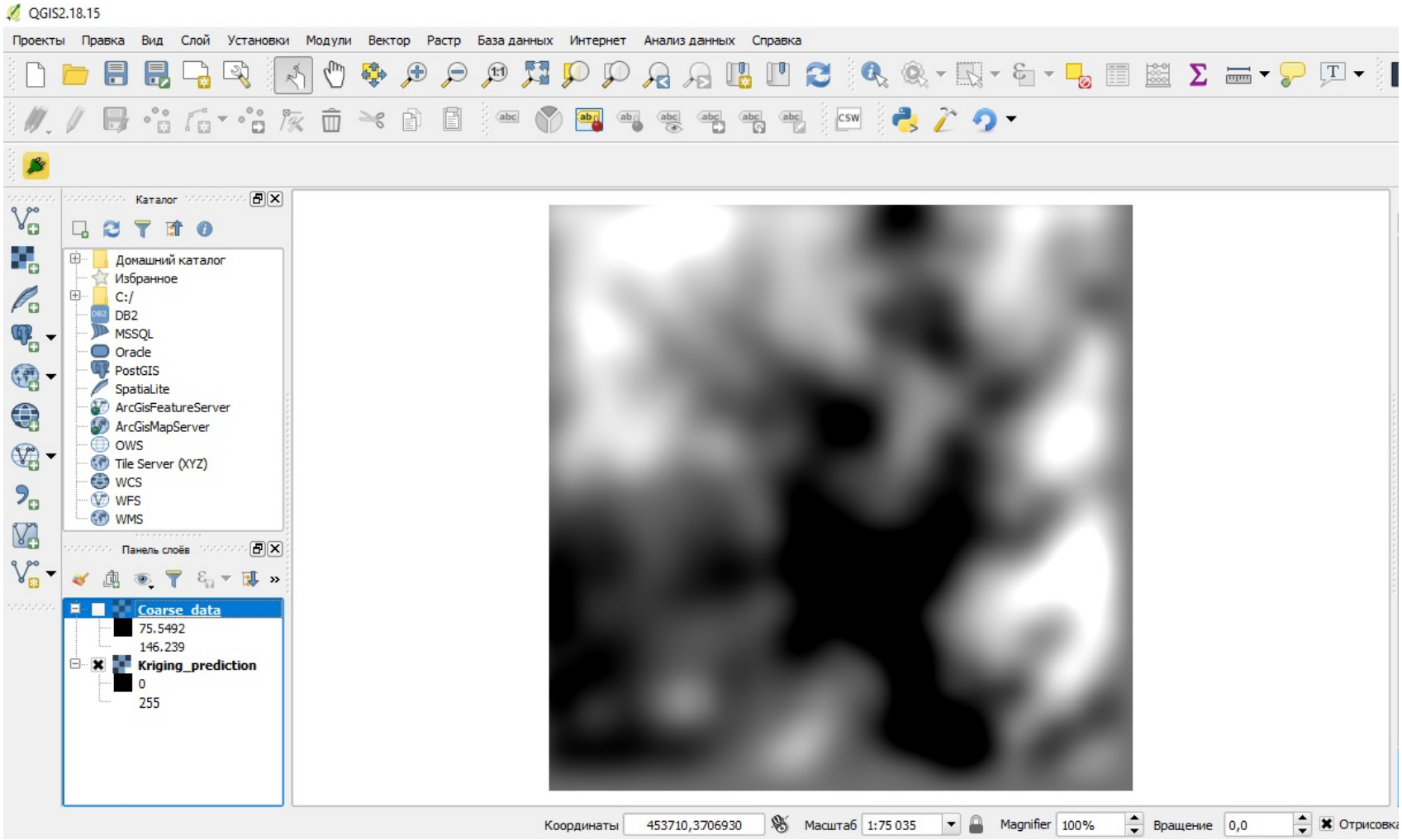
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Performance

- In theory, the speed must asymptotically be higher ($O(n \log n)$ per iteration versus $O(n^2)$)
- But for smaller n writing down the matrix explicitly and solving the system is faster (likely due to complicated structure of `LinearOperator`)
- However, for bigger n the naive implementation just runs out of memory for storage

Summary

- Gaussian regression aka kriging is a technique for interpolating large data sets while using fewer points
- When data is sampled evenly, the matrix for kriging is block Toeplitz with Toeplitz block, which enables faster matrix-vector product and memory-efficient storage
- We implemented the fast kriging algorithm in Python
- The code was converted into a plugin for QGIS

Thank you for your attention!