Recap: Optimization Techniques

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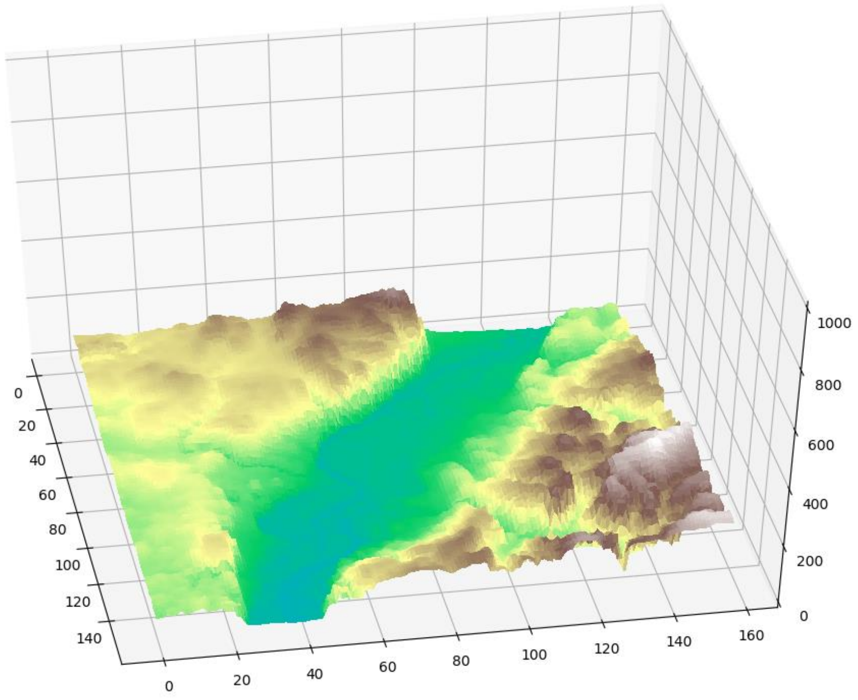

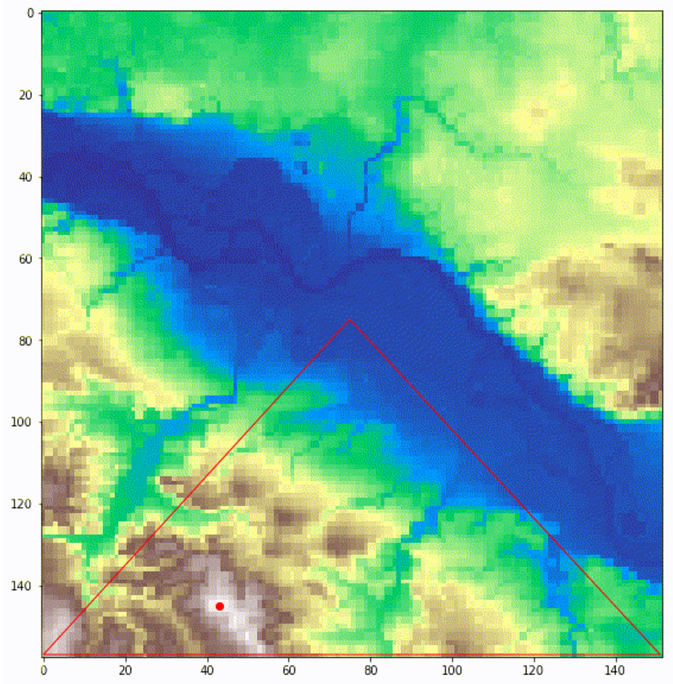

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Regression

Programming for Data Science

Ordinary Least Squares (OLS)

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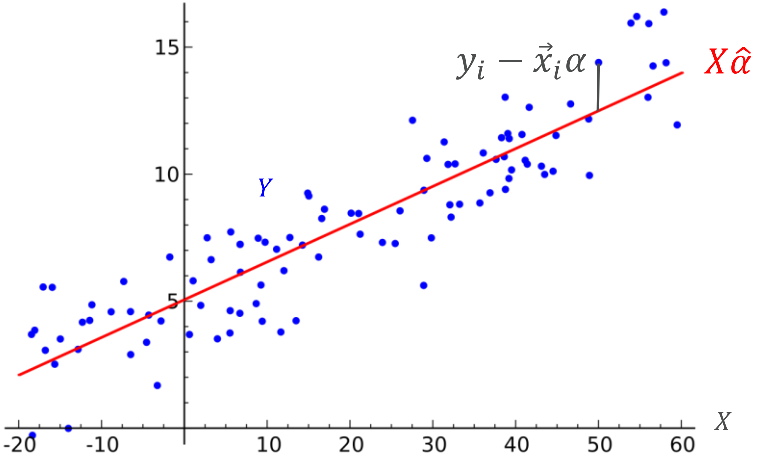
Estimator for linear regression based on minimizing the sum of squared errors (SSE) for a set of observations $X = \{\vec{x}_1, \dots, \vec{x}_n\}$ with $\vec{x}_i = (x_{i1}, \dots, x_{id})$ and values $Y = \{y_1, \dots, y_n\}$

- X: independent variable, Y: dependent variable, α: regression coefficients
- Linear model: $y_i = \alpha_1 \mathrm{x}_{i1} + \alpha_2 x_{i2} + \cdots + \alpha_d x_{id}$ or $y_i = \vec{x}_i \alpha^T$ with $\alpha = (\alpha_1, \dots, \alpha_d)$

$$\hat{\alpha} = \underset{\alpha}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - \vec{x}_i \alpha^T)^2$$



Ordinary Least Squares (OLS)

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Given $X = \{\vec{x}_1, \dots, \vec{x}_n\}$ with $\vec{x}_i = (x_{i1}, \dots, x_{id})$ and $Y = \{y_1, \dots, y_n\}$

- X: independent variable, Y: dependent variable, α: regression coefficients, $\hat{\alpha}$: coefficient estimator
- SSE: Sum of squared errors
- Minimization problem has unique solution (if all d features are linear independent):

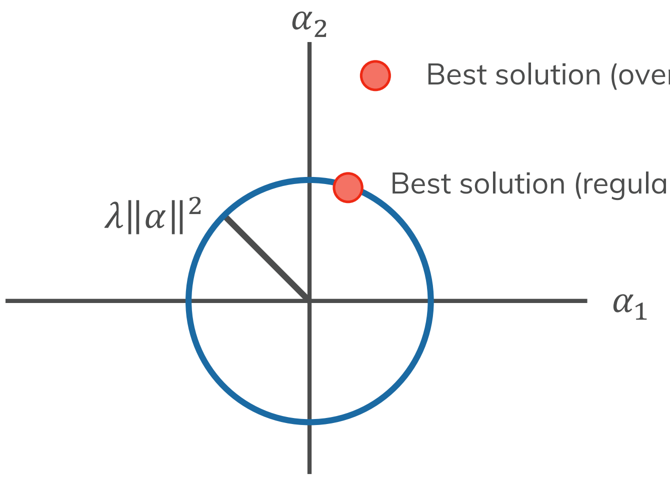
$$\begin{aligned}
\hat{\alpha} &= \underset{\alpha}{\operatorname{argmin}}\, SSE \\
&= \underset{\alpha}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - \vec{x}_i \alpha^T)^2 \\
&= (X^T X)^{-1} X^T Y^T
\end{aligned}$$

Ridge Regression

Introduces regularization for regression models

- OLS is prone to overfitting and underfitting
- Idea: Prefer a certain solution for α with limited variation
- $\underset{\alpha}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - \vec{x}_i \alpha^T)^2 + \lambda \sum_{j=1}^{d} \alpha_j^2$

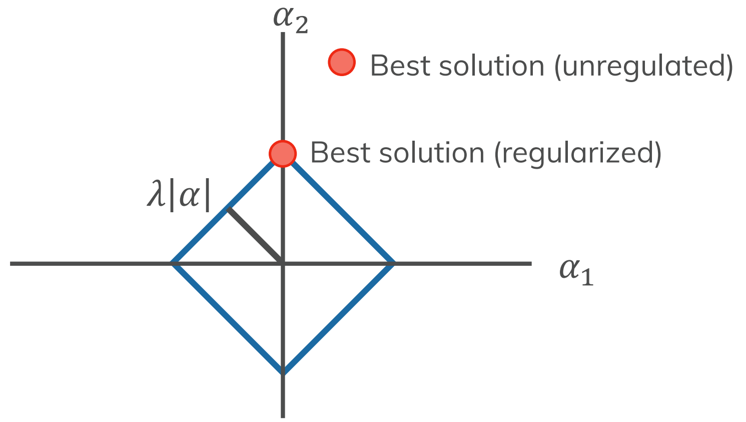
Example for $j \in \{1,2\}$



More Regularization

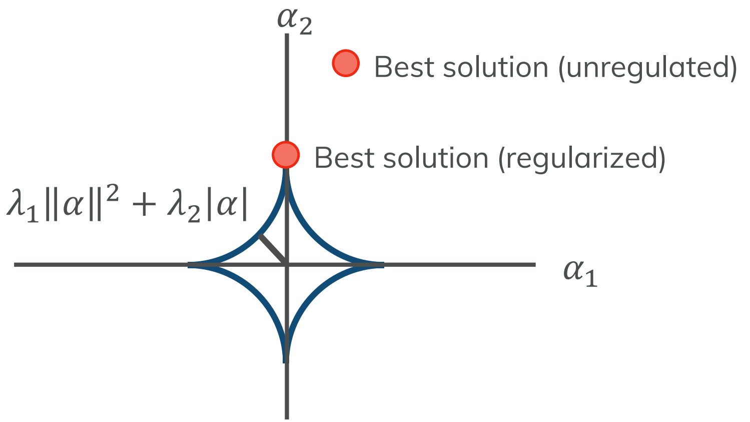
Lasso Regression

- $\underset{\alpha}{\operatorname{argmin}} \sum_{i=1}^{n}(y_i - \vec{x}_i\alpha^T)^2 + \lambda \sum_{j=1}^{d}|\alpha_j|$
- advantage: some α_i can be 0 (feature reduction)



Elastic Net

- $\underset{\alpha}{\operatorname{argmin}} \sum_{i=1}^{n}(y_i - \vec{x}_i\alpha^T)^2 + \lambda_1 \sum_{j=1}^{d}\alpha_j^2 + \lambda_2 \sum_{j=1}^{d}|\alpha_j|$
- advantage: even more α_i can be 0



Task

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Step 0

- You will get a csv file from us. Load it in your language/environment.
- Explore the data in it.

Step 1

- Implement a function* for OLS using optim/minimize.
- Find $\hat{\alpha} = (\mathrm{m}, \mathrm{n}), \mathrm{y_i} = \mathrm{mx_i} + \mathrm{n}$

Step 2

- Implement a function* for OLS using the matrix solution.
- Find $\hat{\alpha}$ and compare its run time to your other OLS function

Step 3

- Implement Ridge, Lasso, and Elastic Net regression* using optim/minimize.
- Compare their resulting $\hat{\alpha}$ to each other and to OLS. Use different values for λ, λ_1, and λ_2.

*use your own implementation

Package suggestions

R

- microbenchmark

python3

- numpy
- scipy
- timeit
- (matplotlib.pyplot)

Exercise Appointment

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We compare and discuss the results

- Tuesday, 12.11.2019,
- Consultation: 07.11.2019,
- Please prepare your solutions! Send us your code!

If you have questions, please mail us:

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