# Project 3

clustering, dimensionality reduction, and non-monotonous neurons

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# Task 3.1

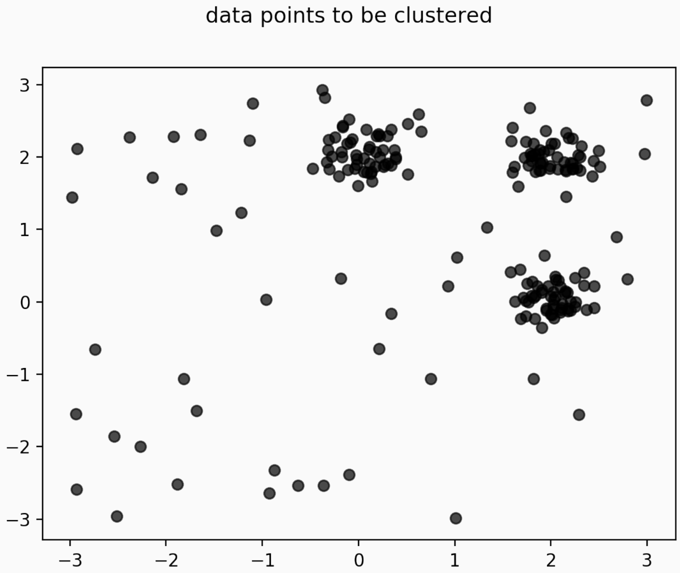
# Fun with k-means clustering

Compare the results and runtimes of three different approaches for k-means clustering:

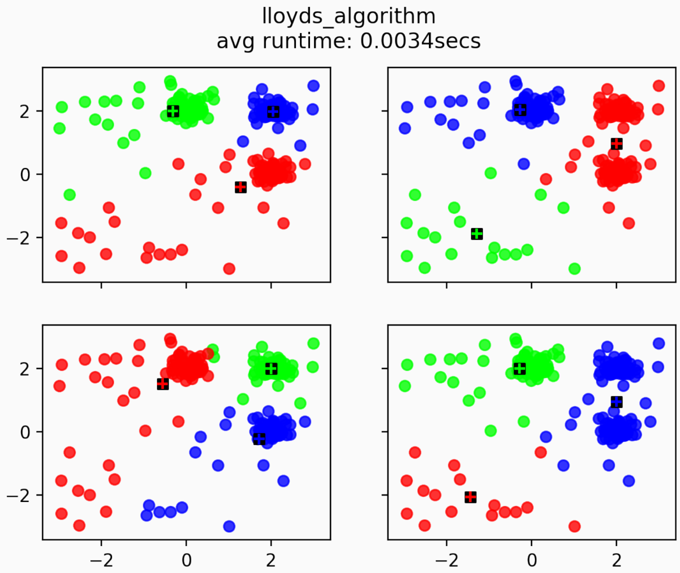
- Lloyd's algorithm
- MacQueen's algorithm
- Hartigan's algorithm

for $k = 3$ clusters.

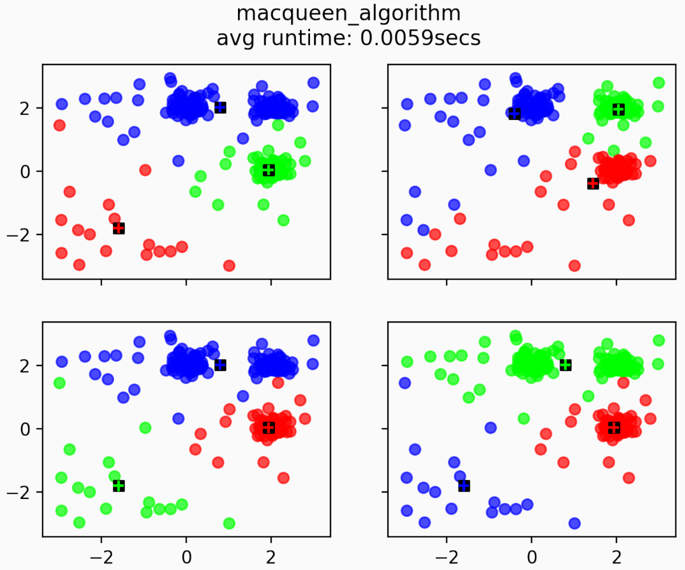
# Given data set



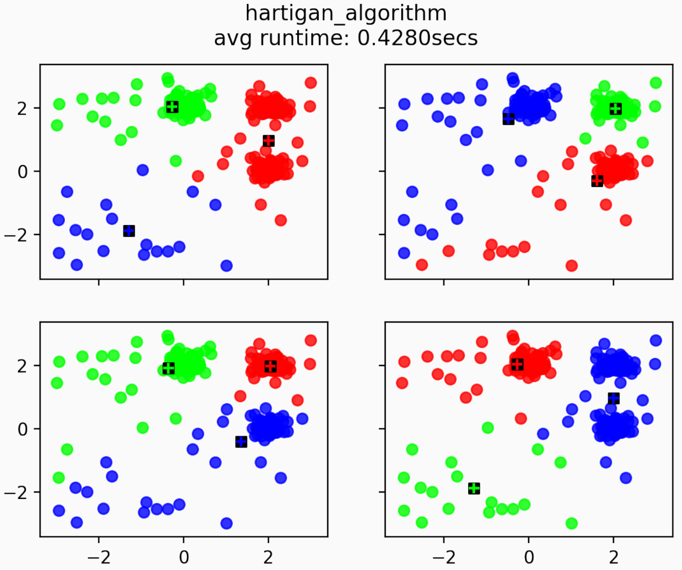
# Lloyd's algorithm



# MacQueen's algorithm



# Hartigan's algorithm



# Task 3.2

# Spectral clustering

Given data, $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^2$, compute similarity matrix:

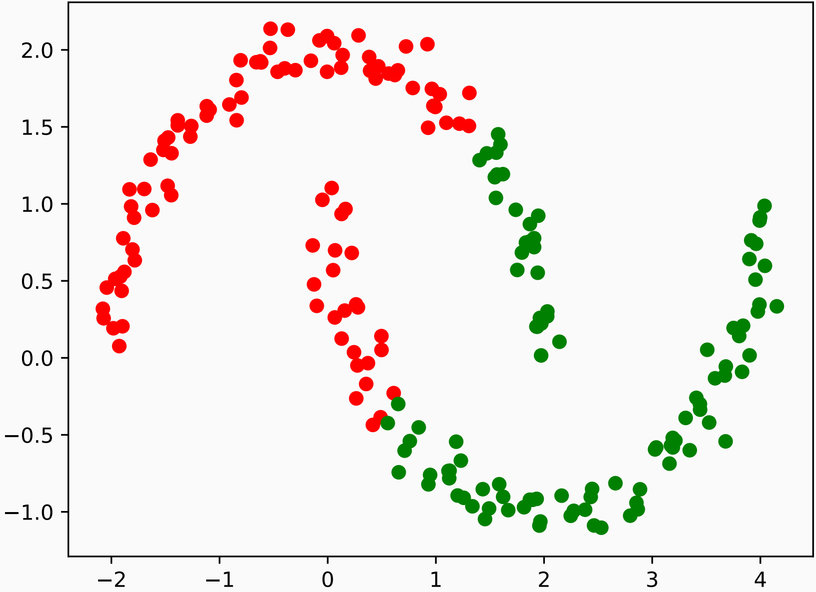
$$S_{ij} = e^{-\beta||x_i - x_j||^2}$$

and the Laplacian $L = D - S$, with diagonal matrix $D$:

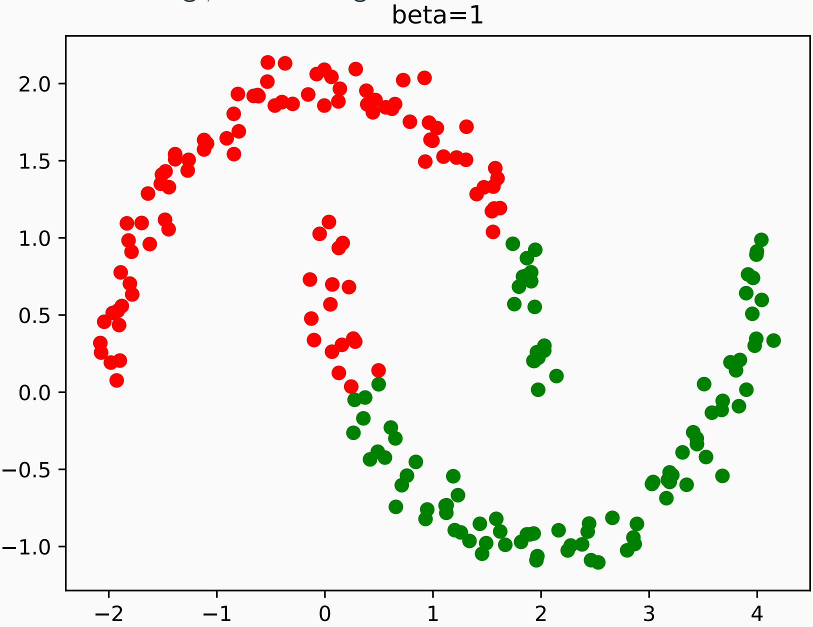
$$D_{ij} = \begin{cases} \sum_j S_{ij} & \text{, if } i = j \\ 0 & \text{, otherwise} \end{cases}$$

Then compute the eigenvalue decomposition of L. Use the eigenvector of the second smallest eigenvalue to partition the data points, according to the sign of the corresponding entry in the eigenvector.

The result using kmeans++:



The result using $\beta = 1$ through 4:



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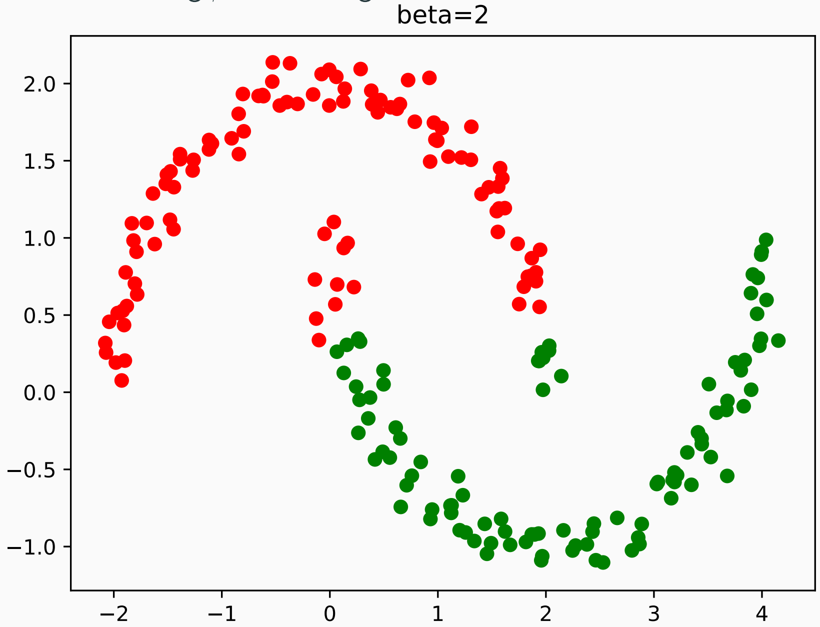

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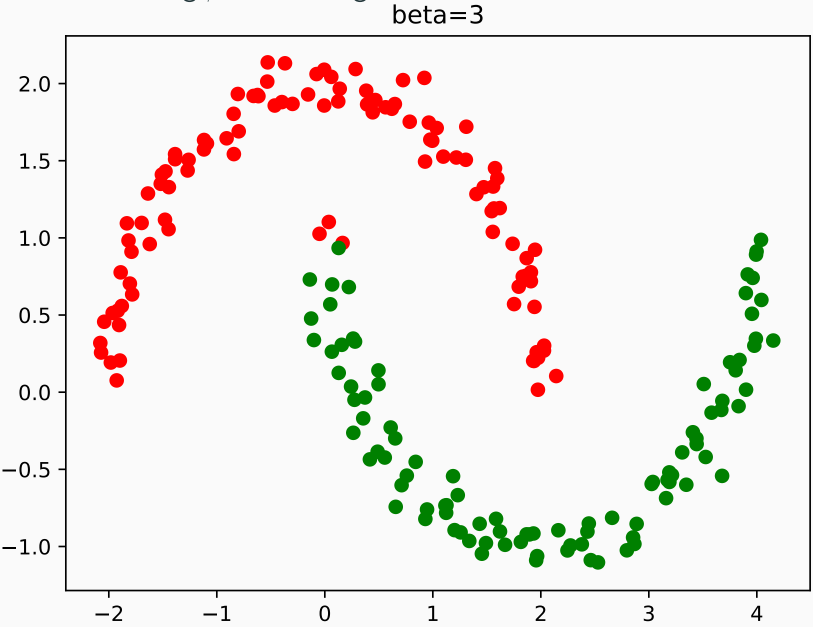

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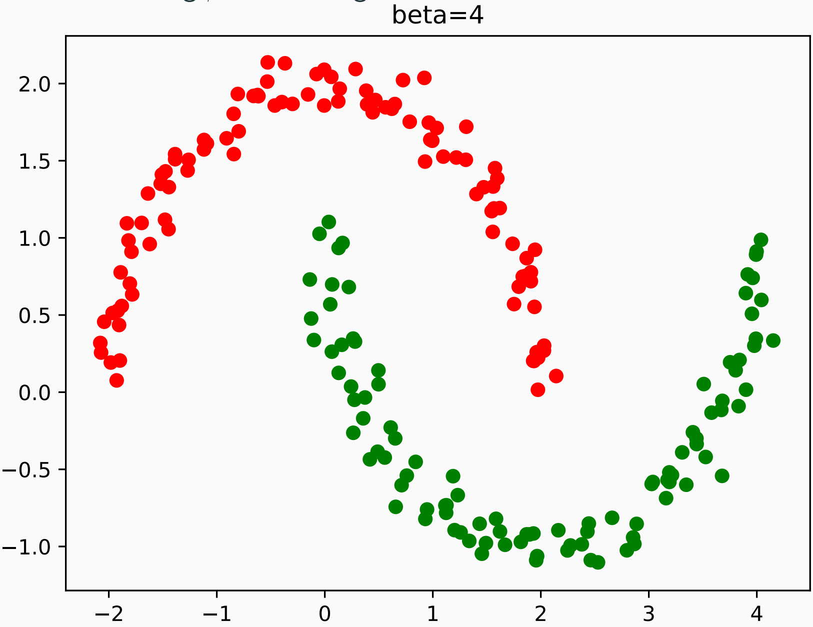


# Task 3.3

# Dimensionality reduction

This task explores mappings $\mathbb{R}^{500} \to \mathbb{R}^2$, in particular Principal Component Analysis (PCA) and multi-class LDA.

# Dimensionality reduction

Idea: Project $n = 150$ *zero-mean* data $x_1, ..., x_n$ onto eigenvectors $u_1$ and $u_2$ corresponding to largest eigenvalues $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$:

PCA: eigenvectors of sample covariance matrix

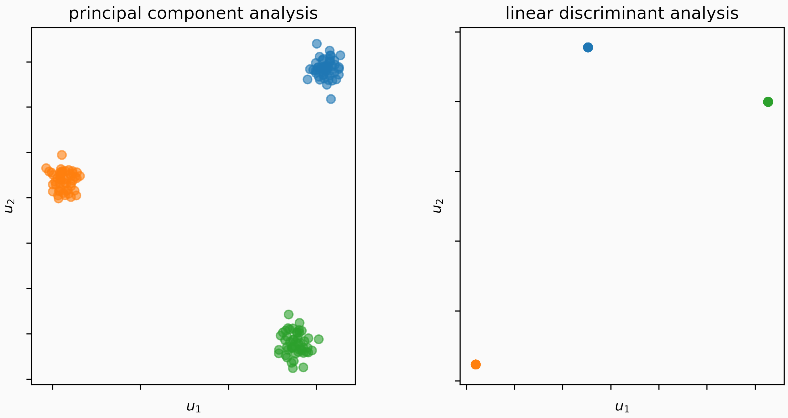
$$\Sigma = \frac{1}{n+1} \sum_{i=1}^{n} x_i \cdot x_i^T$$

LDA: eigenvectors of

$$S_W^{-1} S_B = \left( \sum_{j=1}^{k} \Sigma_j \right)^{-1} \sum_{j=1}^{k} \mu_j \cdot \mu_j^T$$

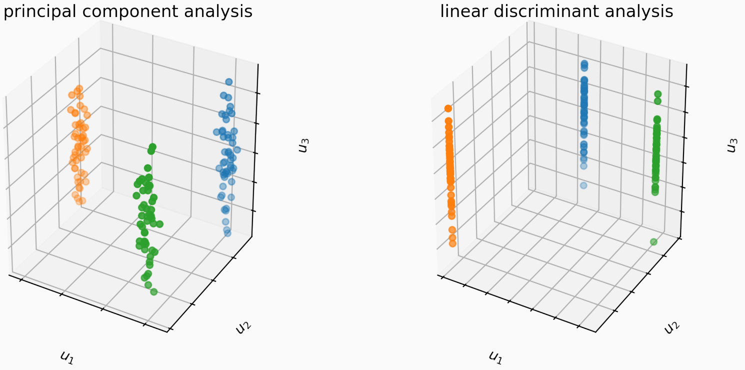
where $\mu_j$ are the mean vectors and $\Sigma_j$ are the covariance matrices for the $k = 3$ classes the data points are from

# PCA and LDA in two dimensions




**Observe:** Data points with same label form clusters if projected.

# PCA and LDA in three dimensions




**Observe:** Data points are (per class) located in a 1D-subspace of $\mathbb{R}^{500}$.

# PCA vs LDA

Why do the results differ?

PCA: Yields axes of maximum variance in complete data set.
$\Rightarrow$ Preserves as much *variance* as possible.

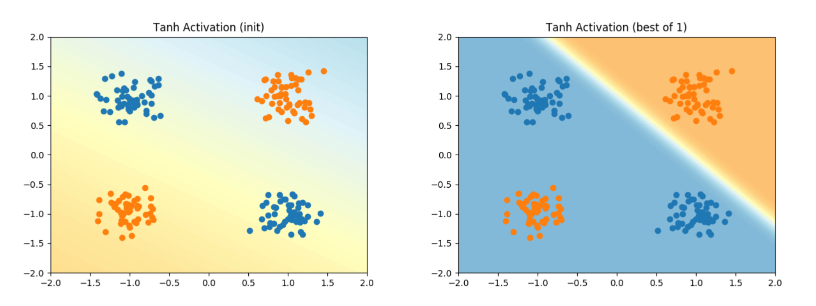
LDA: Uses class labels to maximize distance between class means and minimize class variances.
$\Rightarrow$ Preserves as much *discriminatory* information as possible.

# Task 3.4

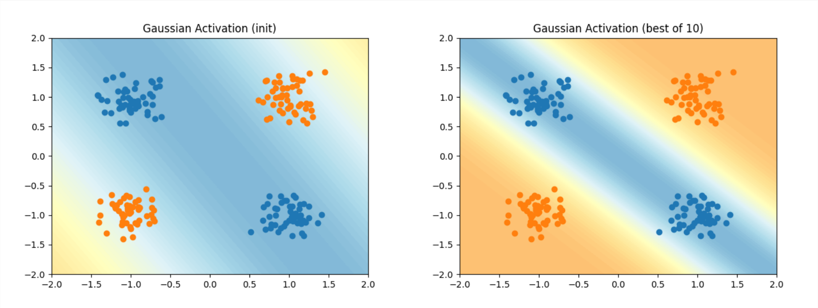
# Perceptrons

- Gradient descent for perceptron learning:
    - line search version
    - use best result of $k$ runs, to prevent local minima
    - monotonous activation separates only linearly
    - avoid this limitation with non-monotonous activation

# Monotonous Perceptron (tanh)



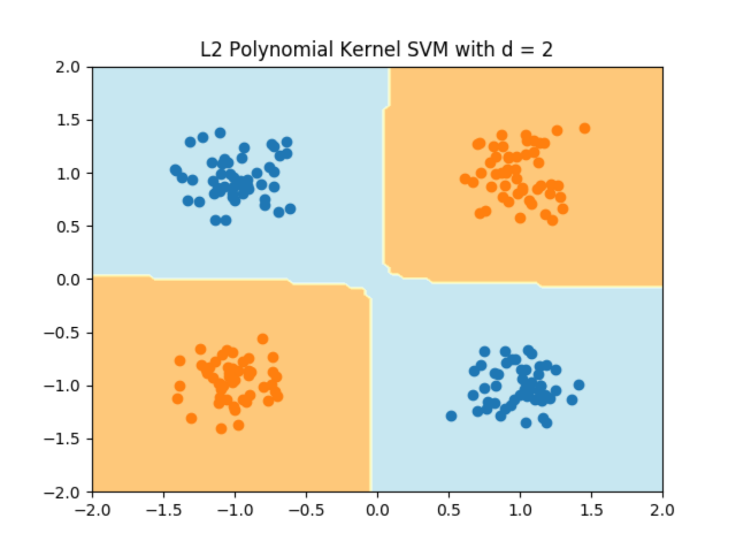
# Non-monotonous Perceptron (Gaussian)



# SVM

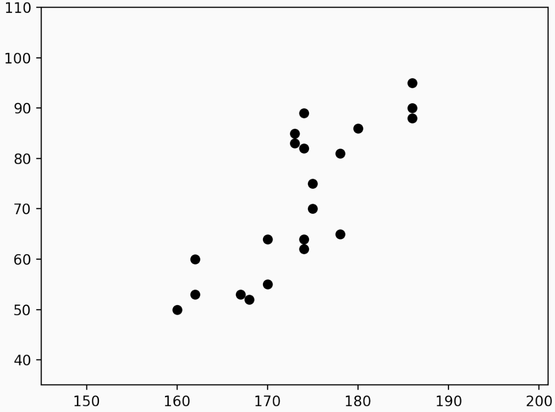
- L2-SVM with polynomial kernel:
    - Train with Frank-Wolfe algorithm
    - $d = 2$ (i.e. quadratic kernel) is enough

# Polynomial Kervel SVM



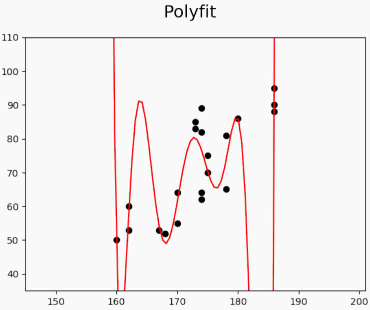
# Task 3.5

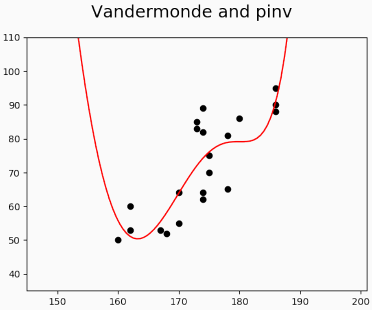
# Exploring numerical instabilities

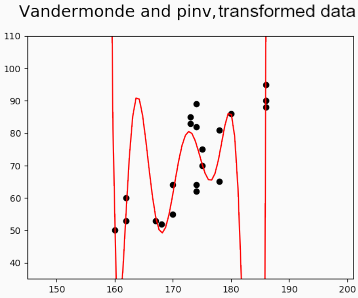


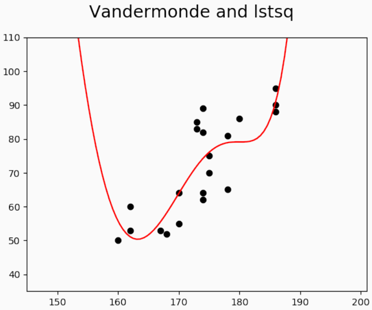

**Task:** Fit a 10th order polynomial to this data using different approaches.

# Resulting fits

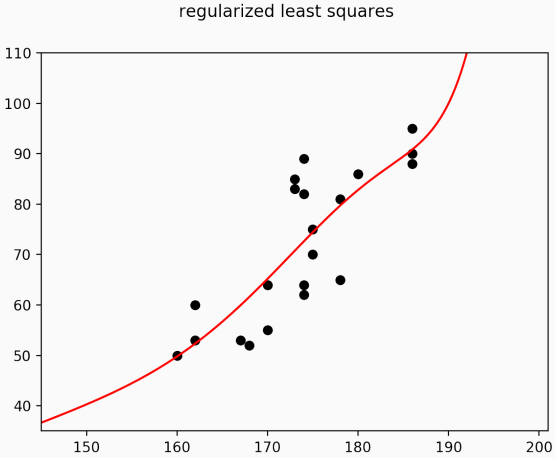


# Regularized least squares




Using Tikhonov-regularization ($\lambda = 0.5$) yields a result that is closer to the more erroneous results from last slide.

Thank you for your attention!