

Foundations of Machine Learning

AI2000 and AI5000

FoML-16
Least Squares for Regression

Dr. Konda Reddy Mopuri
Department of AI, IIT Hyderabad
July-Nov 2025

So far in FoML

- Intro to ML and Probability refresher
- MLE, MAP, and fully Bayesian treatment
- Supervised learning
 - a. Linear Regression with basis functions (regularization, model selection)
 - b. Bias-Variance Decomposition (Bayesian Regression)
 - c. Decision Theory - three broad classification strategies
 - Probabilistic Generative Models - Continuous & discrete data
 - Discriminant Functions



Least Squares for Classification



ભારતીય નોંકેટિક વિજ્ઞાન સંસ્કૃત પ્રોફરાબાદ
ભારતીય પ્રૌદ્યોગિકી સંસ્થાન હૈદરાબાદ
Indian Institute of Technology Hyderabad



Least Squares for Classification

- Consider K classes
- Each class 'k' has its own linear model

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$$



Least Squares for Classification

- Shorter notation $y(\mathbf{x}) = \widetilde{\mathbf{W}}^T \tilde{\mathbf{x}}$

$$\widetilde{\mathbf{W}} =$$

Assign \mathbf{x} to C_k , where

$$\tilde{\mathbf{x}} =$$

$$y(\mathbf{x}) =$$



Least Squares for Classification

- Data matrix
- Target matrix

Use regression (sum of squares) error function

$$E_D(\tilde{\mathbf{W}}) =$$



Least Squares for Classification

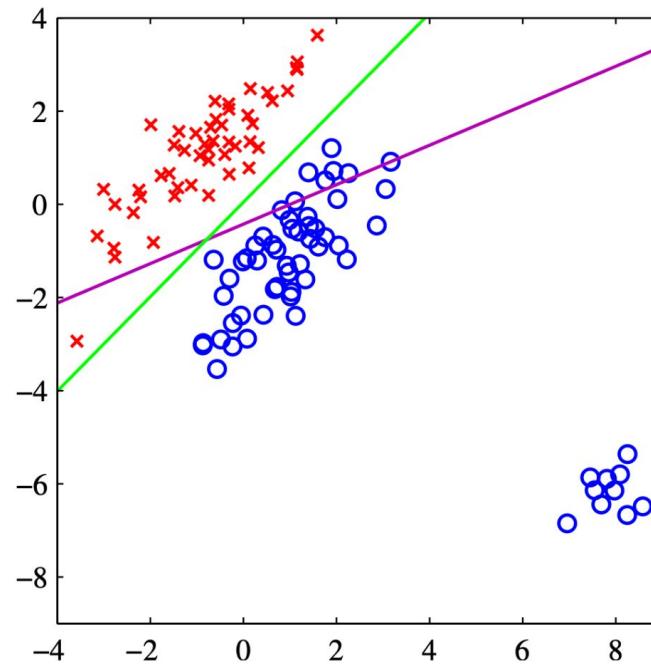
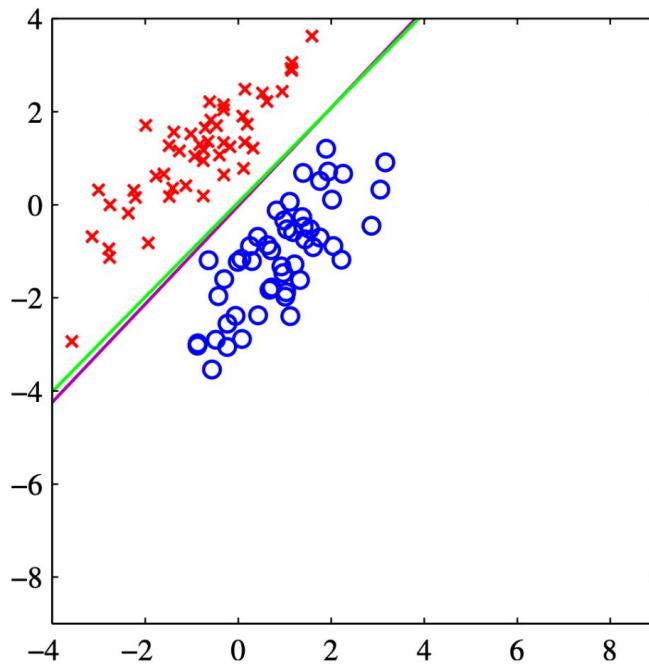
The error function can be conveniently written as

$$E_D(\tilde{\mathbf{W}}) = \frac{1}{2} \text{Tr} \left\{ (\tilde{\mathbf{X}}\tilde{\mathbf{W}} - \mathbf{T})^T (\tilde{\mathbf{X}}\tilde{\mathbf{W}} - \mathbf{T}) \right\}$$

Minimize $E_D(\tilde{\mathbf{W}})$ as a function of $\tilde{\mathbf{W}}$:



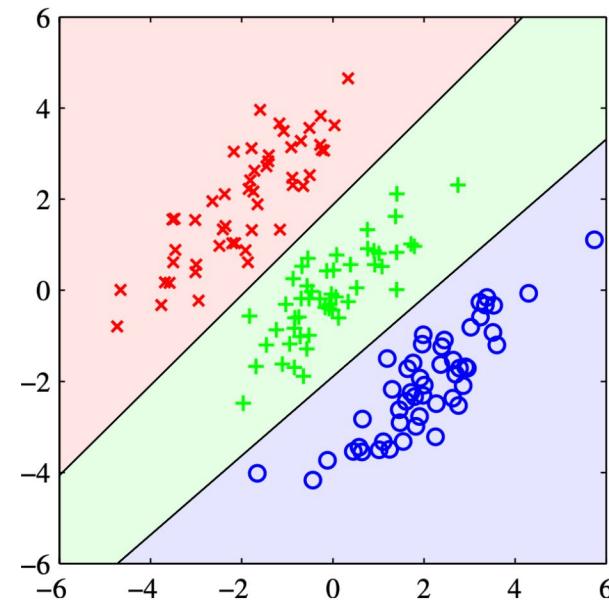
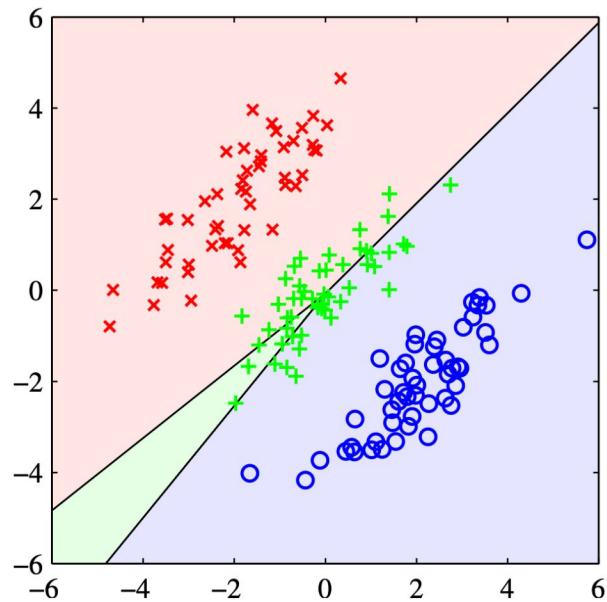
Least Squares Issues - Outliers



ભારતીય સૌંકેટિક વિજ્ઞાન સંસ્કૃતી
ભારતીય પ્રોફોગિકી સંસ્થાન હૈદરાબાદ
Indian Institute of Technology Hyderabad

Magenta - LS classifier
Green - Logistic Regression classifier

Least Squares Issues - Masking



Left - LS classifier
Right - Logistic Regression classifier



ભારતીય નોકેપિક વિજ્ઞાન સંસ્કૃતિકા
ભારતીય પ્રૌદ્યોગિકી સંસ્થાન હૈદરાબાદ
Indian Institute of Technology Hyderabad

DIL

Data-driven Intelligence
& Learning Lab

Least Squares Issues - Predictions * Probabilities

$\mathbf{y}_{LS}(\mathbf{x})$ are not probabilities



ભારતીય નોંકેટિક વિજ્ઞાન સંસ્કૃત પ્રેરણાખાડ
ભારતીય પ્રૌદ્યોગિકી સંસ્થાન હૈદરાબાદ
Indian Institute of Technology Hyderabad



Rough



ભારતીય નોંકેટિક વિજ્ઞાન સંસ્કૃત પ્રૌદ્યોગિક
ભારતીય પ્રૌદ્યોગિકી સંસ્થાન હૈદરાબાદ
Indian Institute of Technology Hyderabad



Next The Perceptron



ભારતીય નોંકેટિક વિજ્ઞાન સંસ્કૃત પ્રેરણાખાડ
ભારતીય પ્રૌદ્યોગિકી સંસ્થાન હૈદરાબાદ
Indian Institute of Technology Hyderabad

