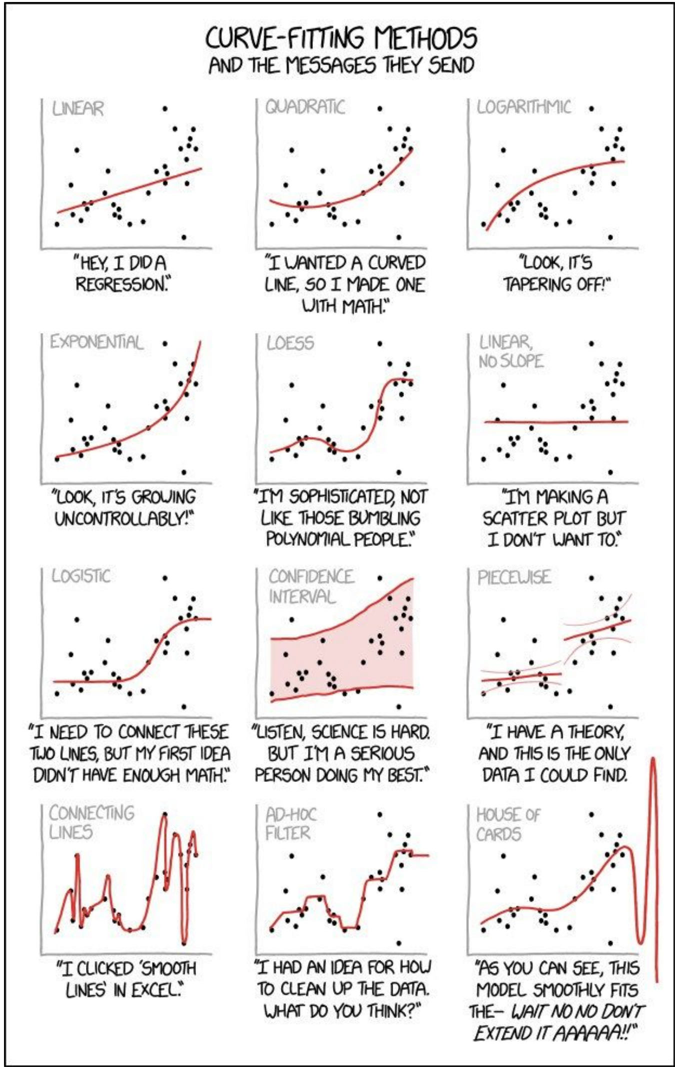
Machine Learning Course

Lecture 2: Linear models

MIPT, 2019

Outline

1. Overview of linear models.
2. Linear regression.
3. Analytical solution.
4. Regularization.
5. Gauss-Markov theorem.
6. Probabilistic interpretation and intuition.


CURVE-FITTING METHODS
AND THE MESSAGES THEY SEND
LINEAR
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QUADRATIC
"I WANTED A CURVED LINE, SO I MADE ONE WITH MATH."
LOGARITHMIC
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LOESS
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CONFIDENCE INTERVAL
"LISTEN, SCIENCE IS HARD. BUT I'M A SERIOUS PERSON DOING MY BEST."
PIECEWISE
"I HAVE A THEORY, AND THIS IS THE ONLY DATA I COULD FIND."
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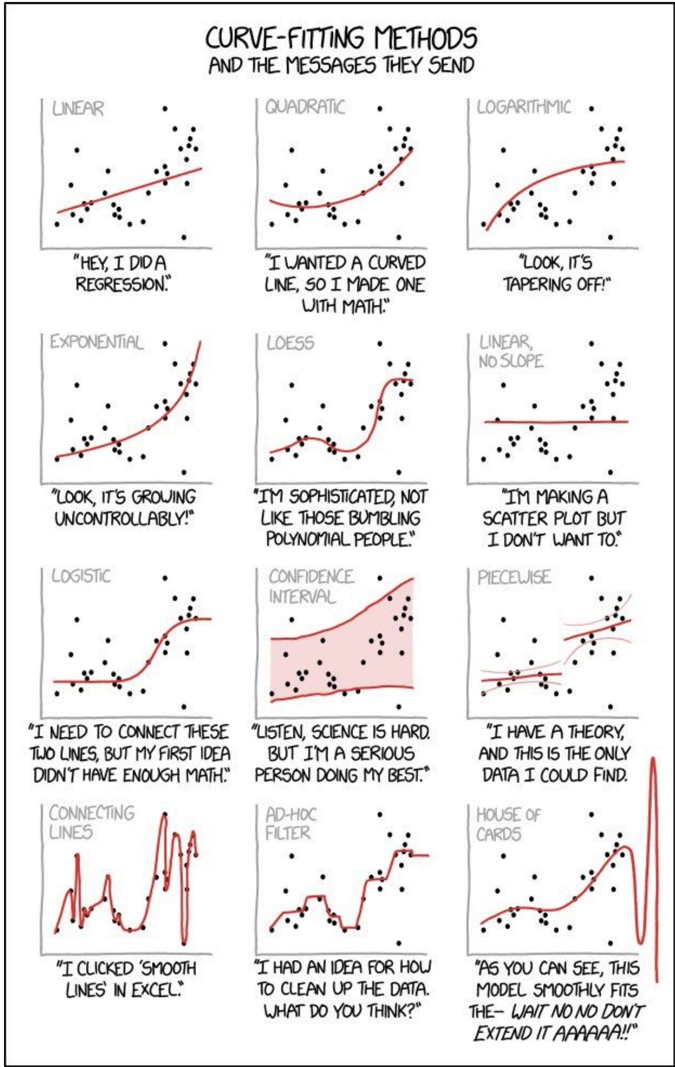
AD-HOC FILTER
"I HAD AN IDEA FOR HOW TO CLEAN UP THE DATA. WHAT DO YOU THINK?"
HOUSE OF CARDS
"AS YOU CAN SEE, THIS MODEL SMOOTHLY FITS THE- WAIT NO NO DON'T EXTEND IT AAAAAA!!"

Example questions linear regression can solve (up right picture):

- What will be my monthly spending for the next year?
- Which factor is more important in deciding my monthly spending?
- How monthly income and trips per month are correlated with monthly spending?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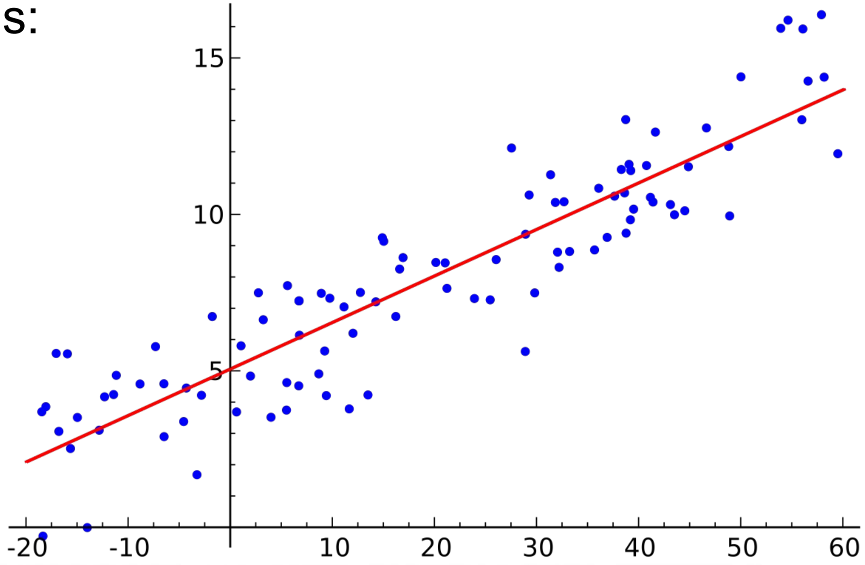
Linear models

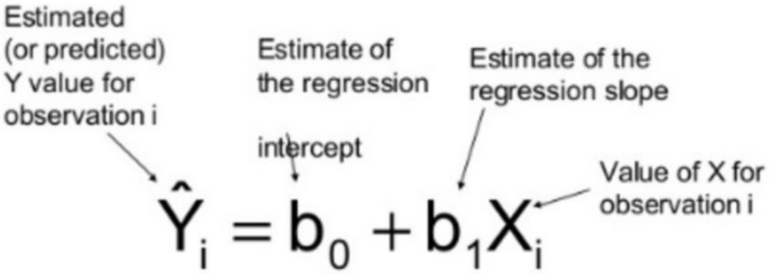
$$\underset{\downarrow}{Y} = \underbrace{X_1 + X_2 + X_3}_{\downarrow}$$

Dependent Variable	Independent Variable
Outcome Variable	Predictor Variable
Response Variable	Explanatory Variable

Linear models

- Predictive models:





Estimated (or predicted) Y value for observation i

Estimate of the regression intercept

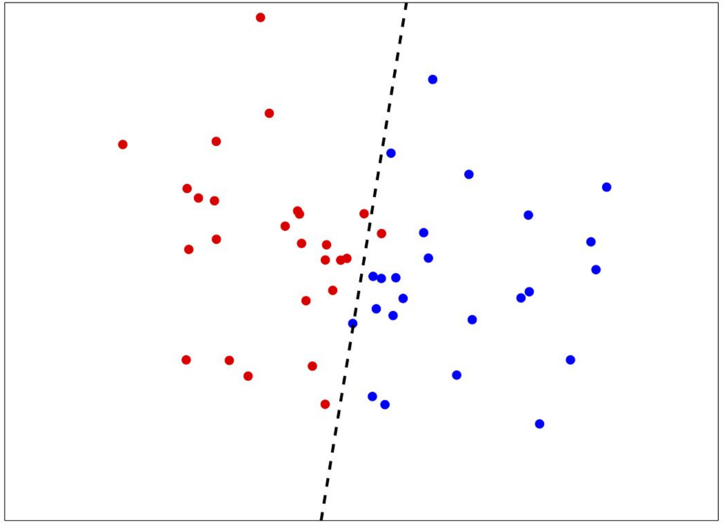
Estimate of the regression slope

Value of X for observation i

$$\hat{Y}_i = b_0 + b_1 X_i$$

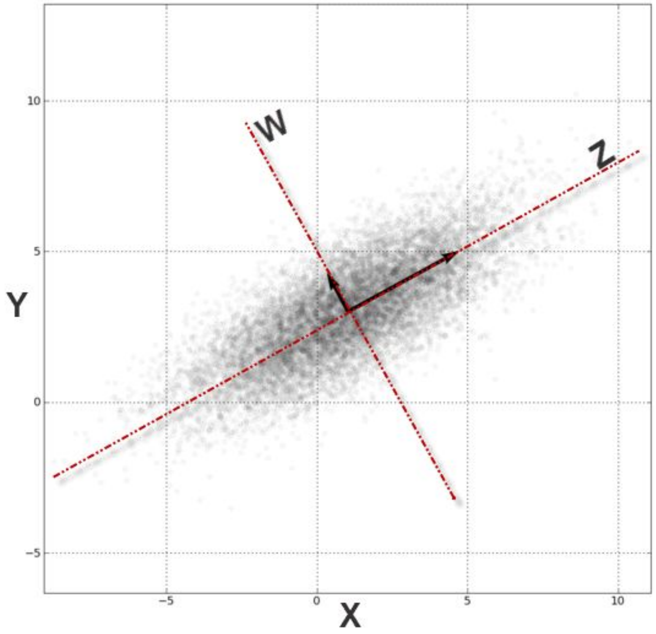
Linear models

- Predictive models:
- Classification models:



Linear models

- Predictive models:
- Classification models:
- Unsupervised models (e.g. PCA analysis)



Linear models

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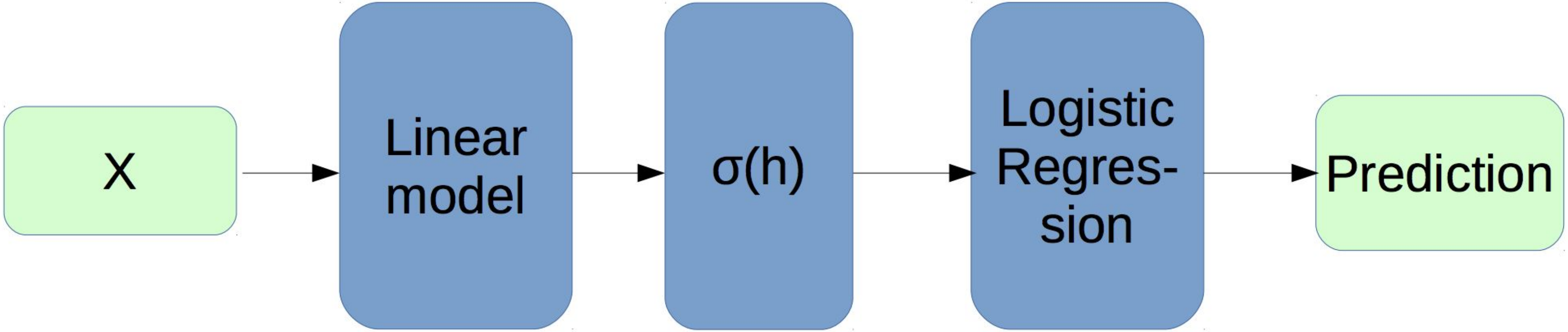
- Building block of other models (ensembles, NNs, etc.)



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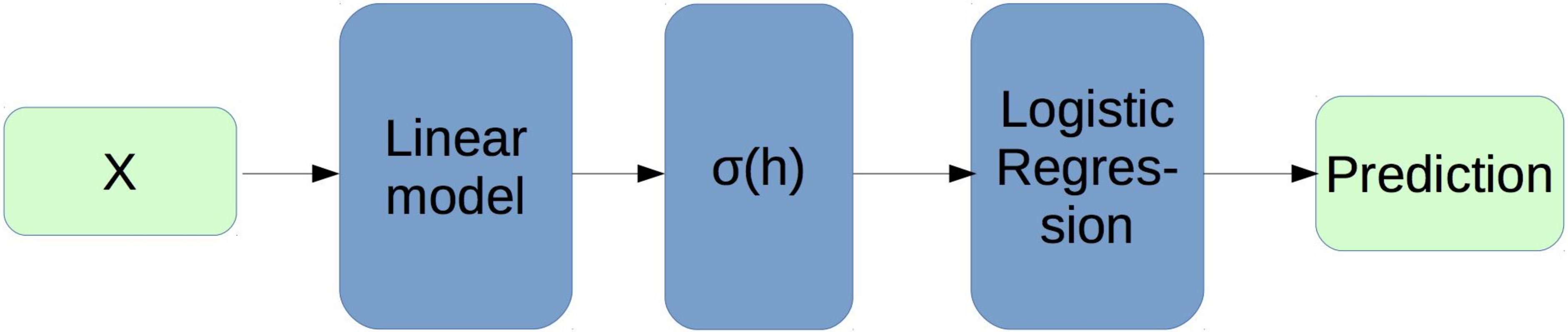

Actually, it’s a neural network. We will meet it later.

Linear regression

Linear regression problem statement:

- Training set $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$, where ($\mathbf{x} \in \mathbb{R}^p$, $y \in \mathbb{R}$) .

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  Where $\mathbf{w} = (w_1, \ldots w_p)$ is weights vector, w_0 is bias term.

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- Least squares method provides a solution:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|\mathbf{w}_0 + (\mathbf{x}_1 \dots \mathbf{x}_n)^T \mathbf{w} - (y_1, \dots, y_n)\|_2^2$$

Analytical solution

Denote quadratic loss function: $Q(\mathbf{w}) = (Y - X\mathbf{w})^T(Y - X\mathbf{w}) = \|Y - X\mathbf{w}\|_2^2$,

where $X = [\mathbf{x}_1, \dots, \mathbf{x}_n], \quad \mathbf{x}_i \in \mathbb{R}^p$, $Y = [y_1, \dots, y_n], \quad y_i \in \mathbb{R}$.

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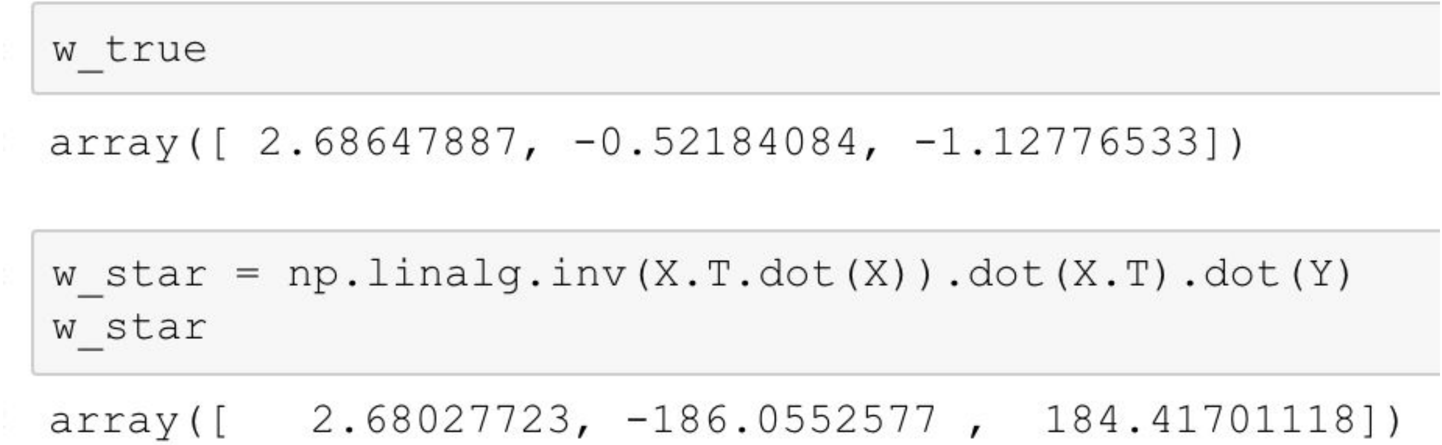
$$\hat{\mathbf{w}} = \boxed{(X^T X)}^{-1} X^T Y$$

what if this matrix is *singular?*

Unstable solution

In case of multicollinear features the matrix X^TX is almost singular .

It leads to unstable solution:



```
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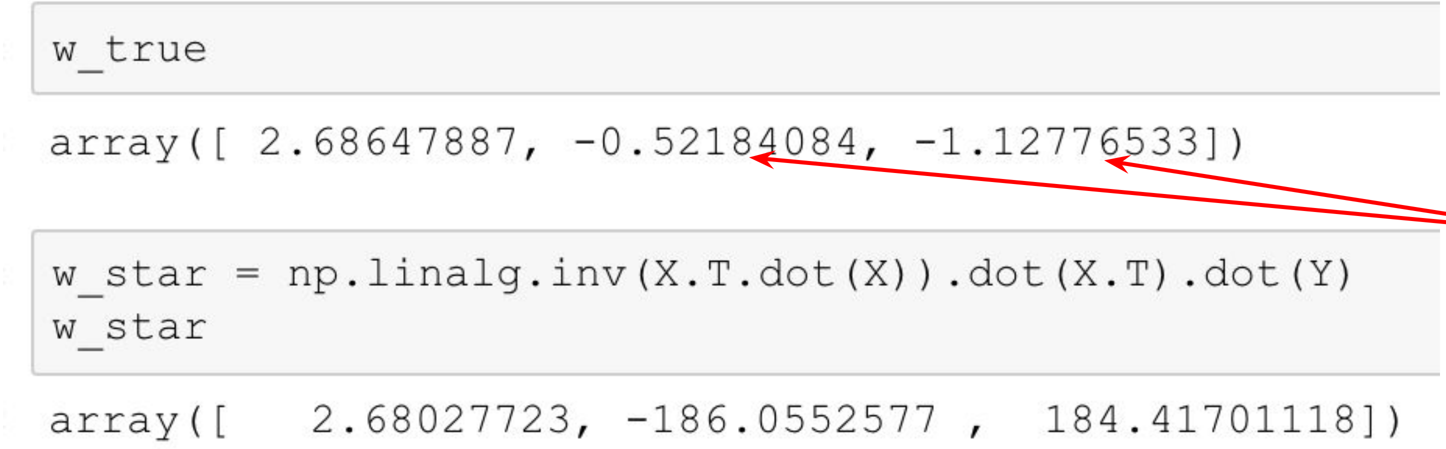

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corresponding features are almost collinear

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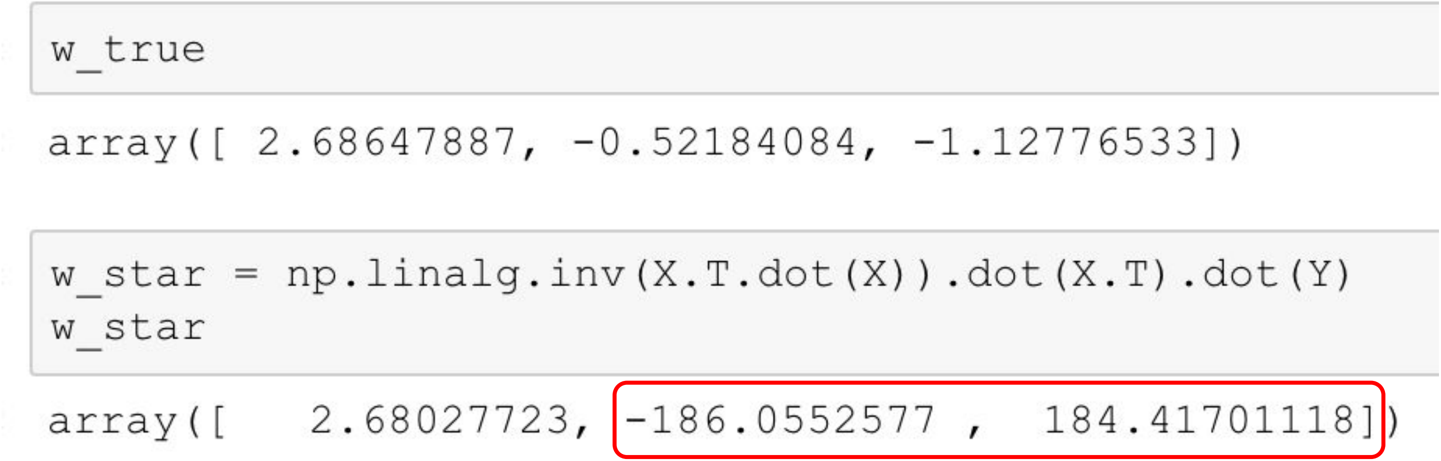

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the coefficients are huge and sum up to almost 0

Regularization

To make the matrix nonsingular, we can add a diagonal matrix:

$$\hat{\mathbf{w}} = (X^T X + \lambda I)^{-1} X^T Y \,,$$

where $I = \mathrm{diag}[1_1, \ldots, 1_p]$.

Actually, it’s a solution for the case $Q(\mathbf{w}) = \|Y - X\mathbf{w}\|_2^2 + \lambda^2 \|\mathbf{w}\|_2^2$.

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exercise: check it by yourself

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Gauss-Markov theorem

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Then the solution $\hat{\mathbf{w}} = (X^T X)^{-1} X^T Y$ delivers BLEU: **B**est **L**inear **U**nbiased **E**stimator.

Different norms

Once more: loss functions:

- $MSE = \frac{1}{n}\|\mathbf{x}^T\mathbf{w} - \mathbf{y}\|_2^2$

Regularization terms:

- L_2: $\|\mathbf{w}\|_2^2$

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only works for Gauss-Markov theorem

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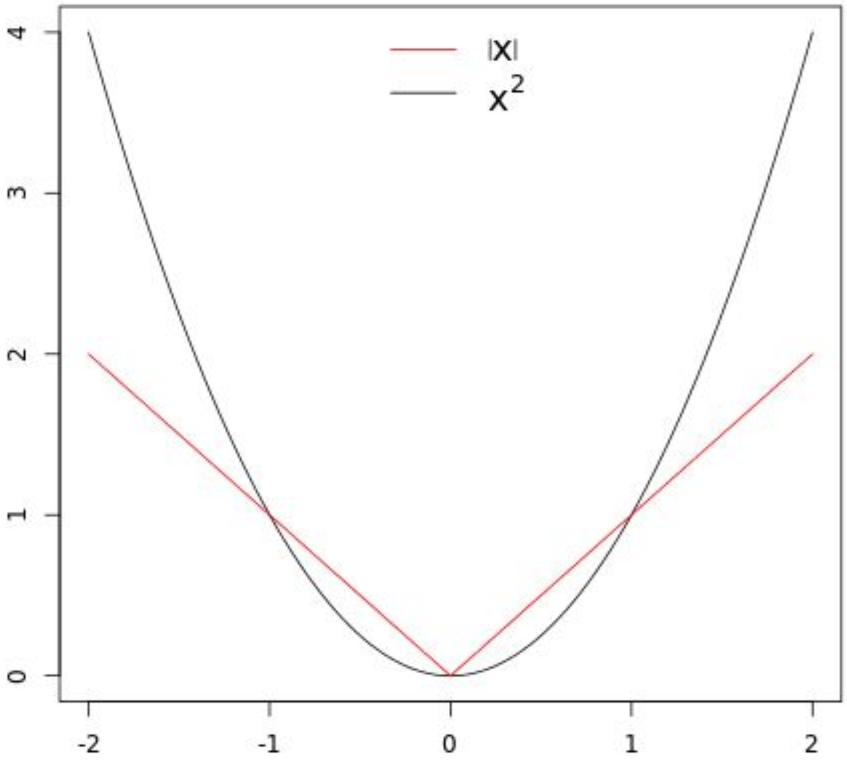

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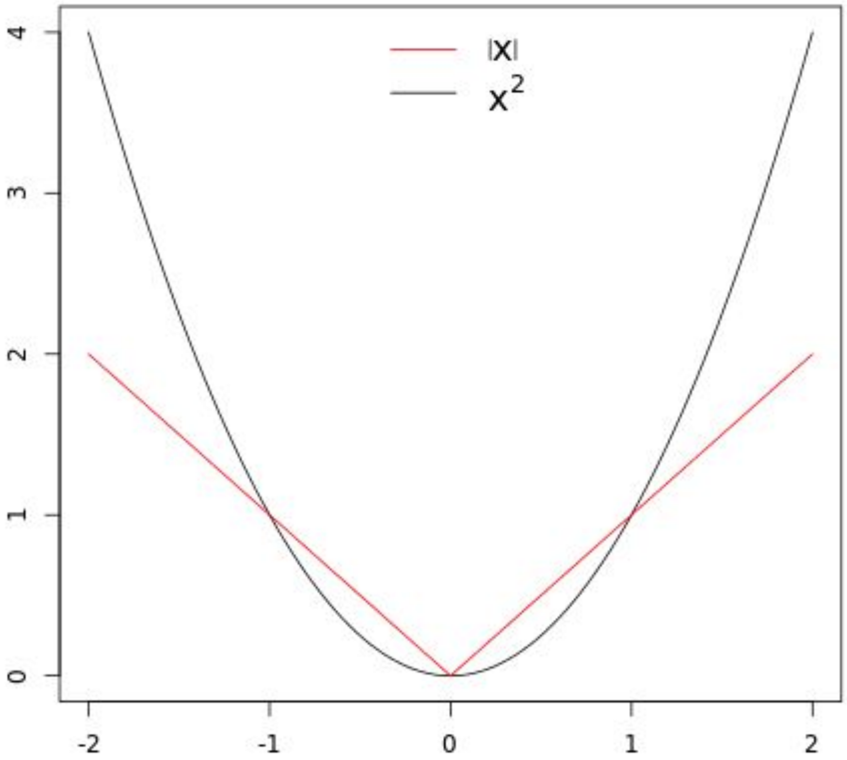

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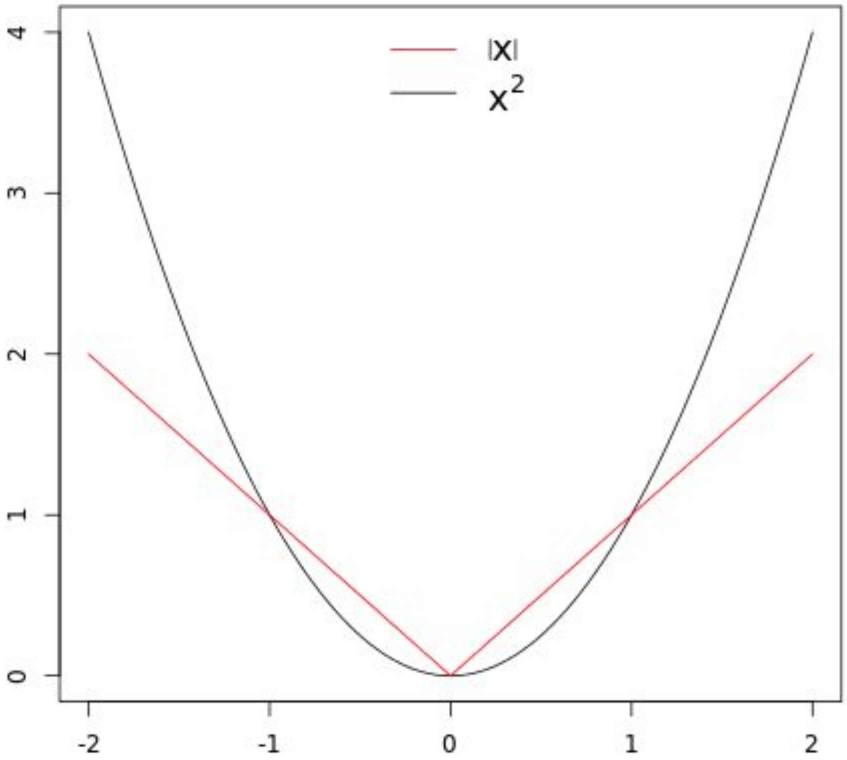

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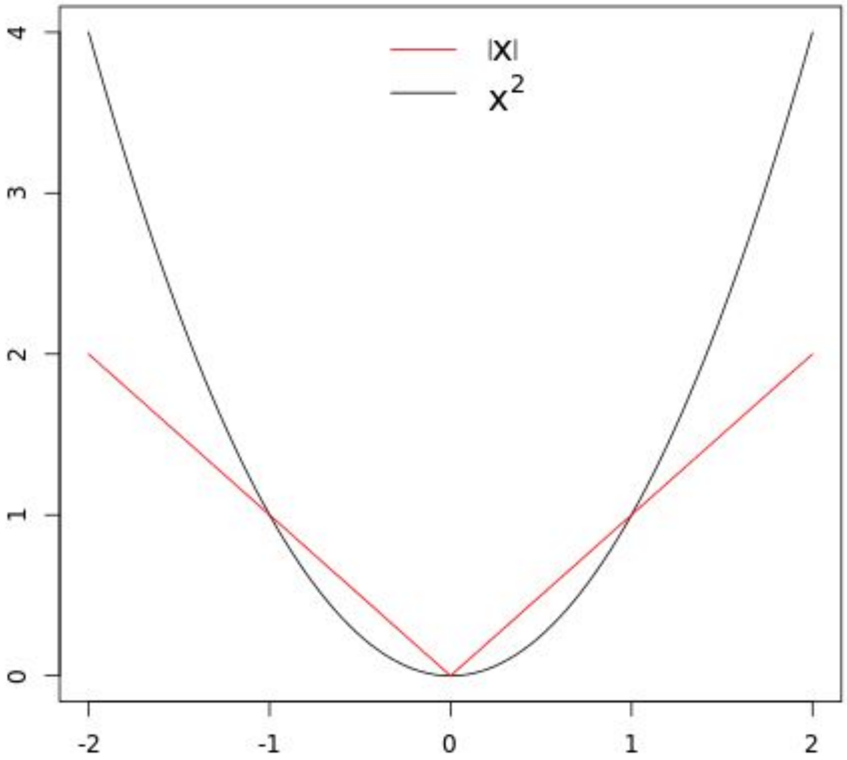

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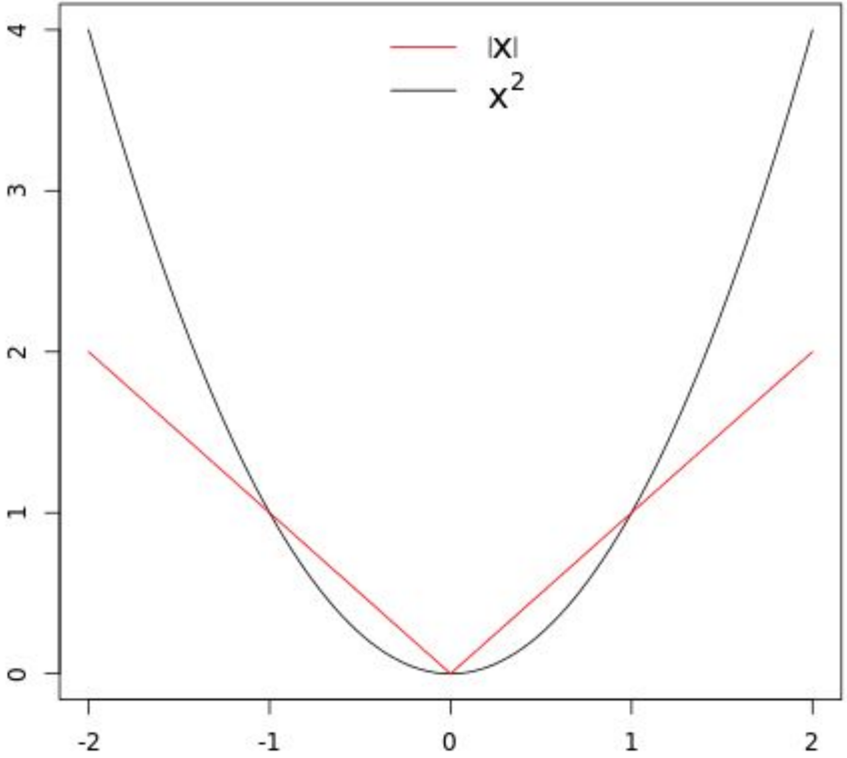

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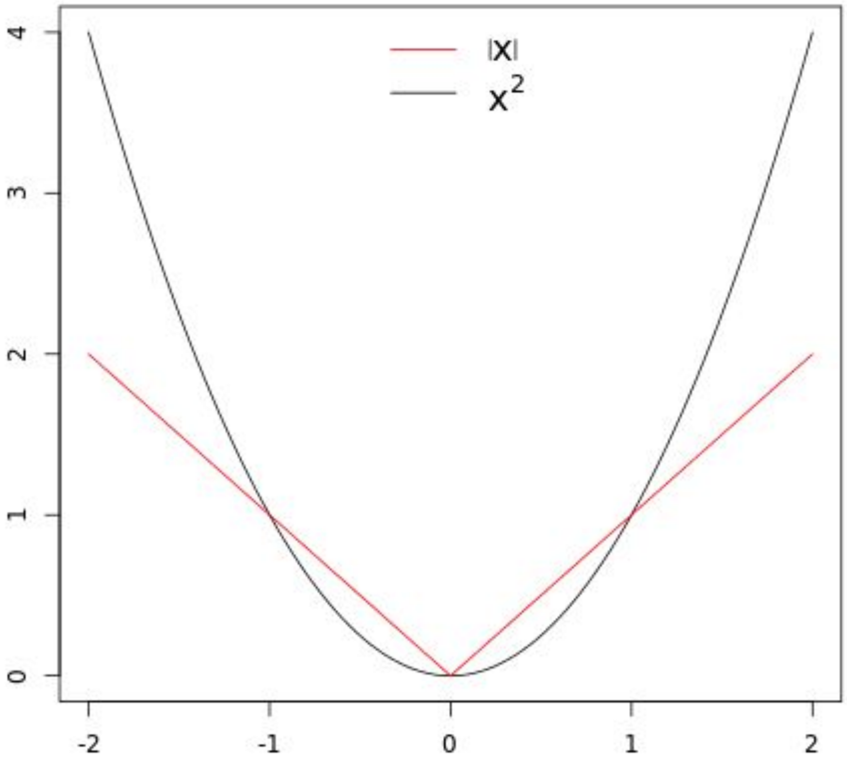
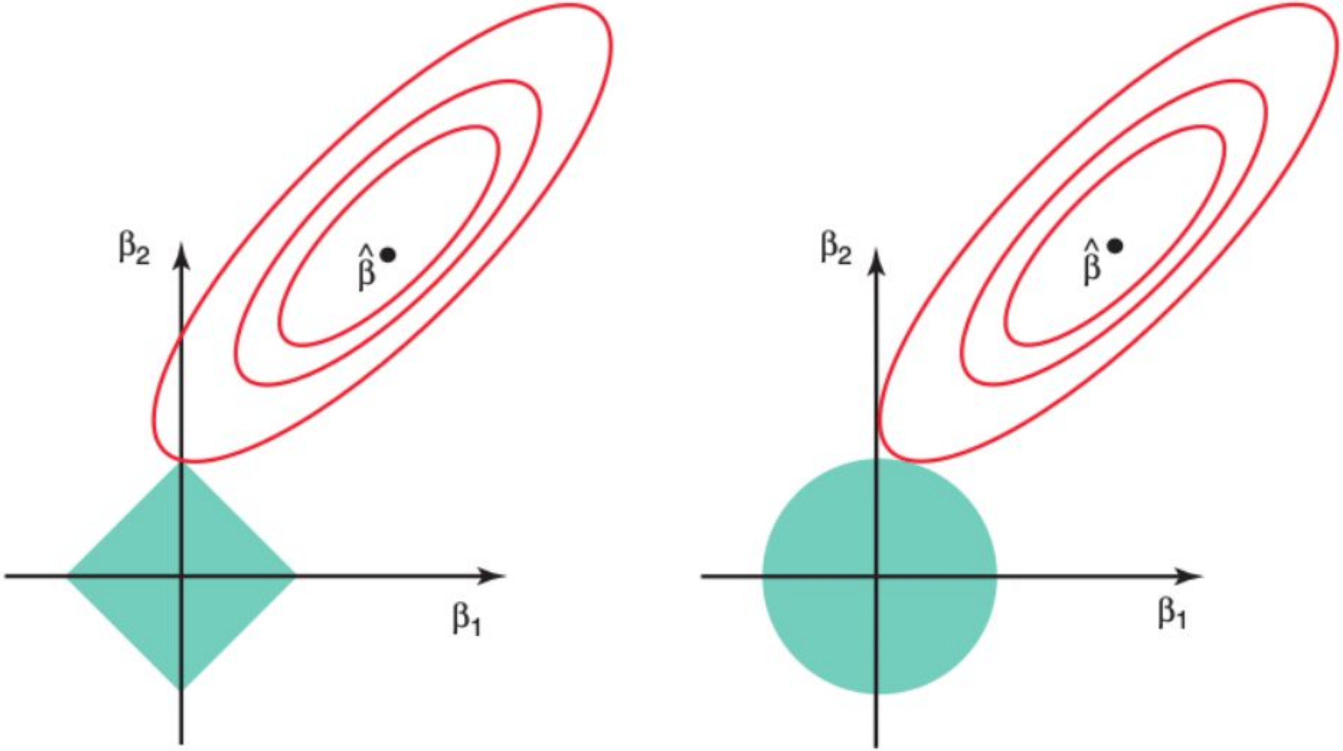
Does what?



Regularization: illustration

$$\mathbf{w} = [\beta_1, \beta_2]$$



source: Modern Multivariate Statistical Techniques

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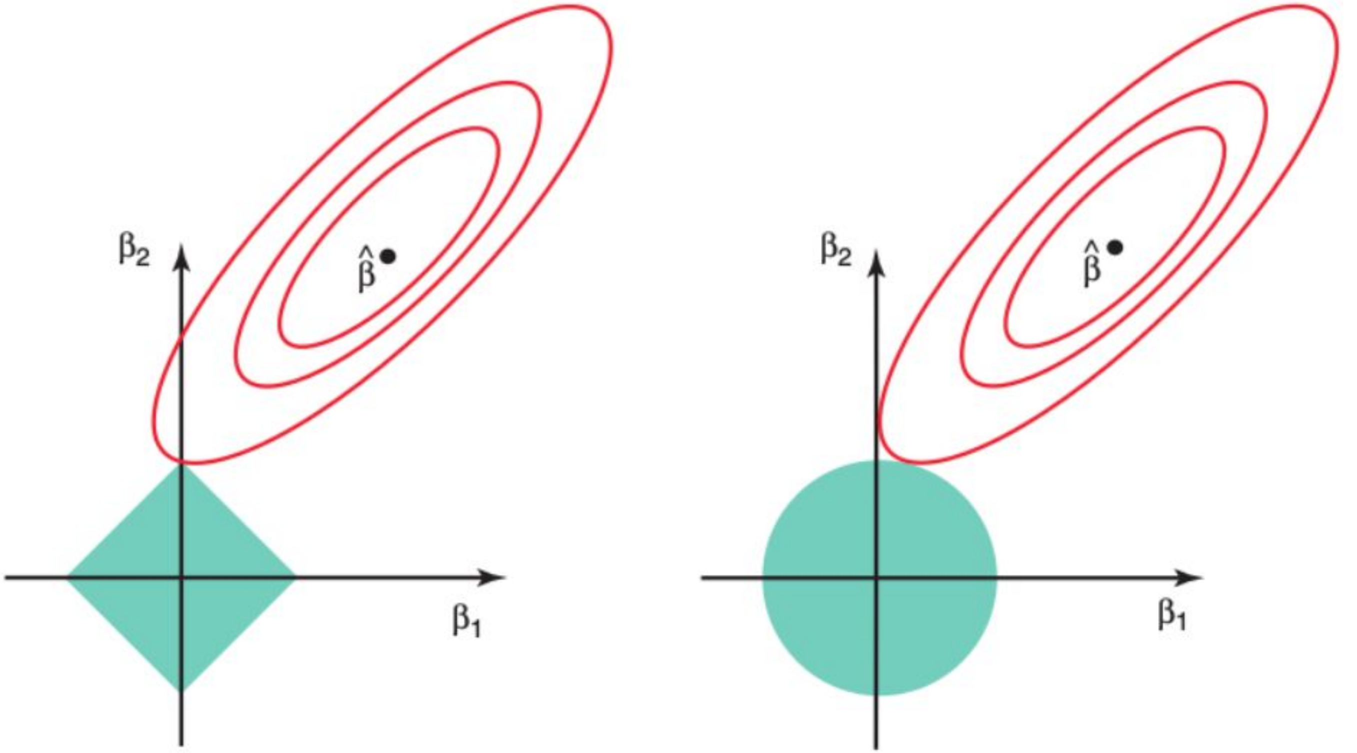


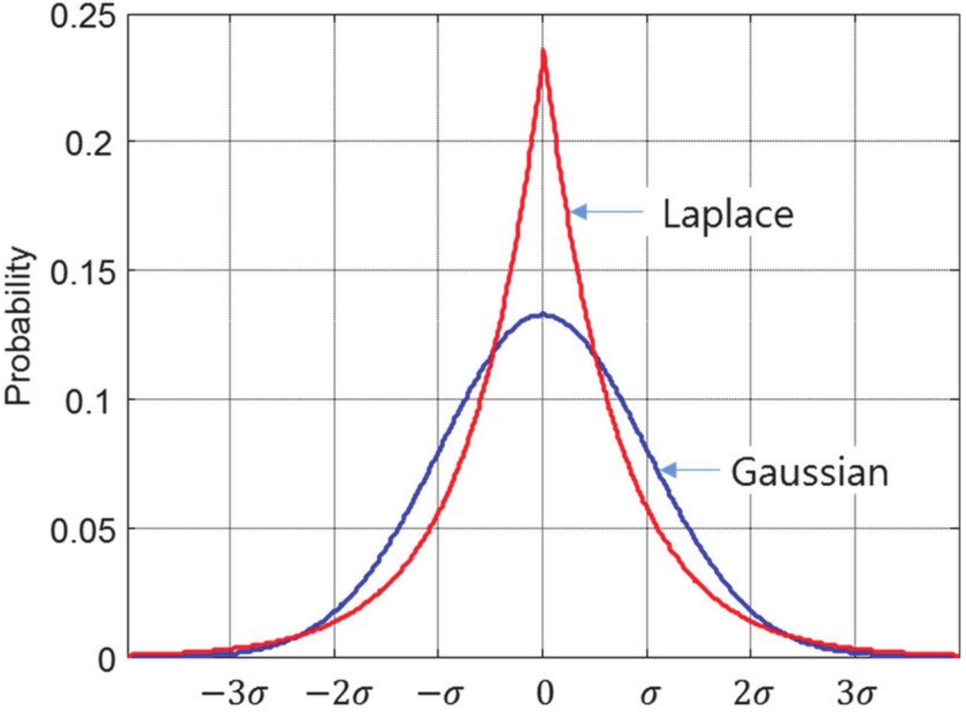
L_1 regularization

L_2 regularization

source: Modern Multivariate Statistical Techniques

Regularization: probability interpretation

assume **w** elements are sampled from some *specific* distribution (prior distribution for the weights vector)



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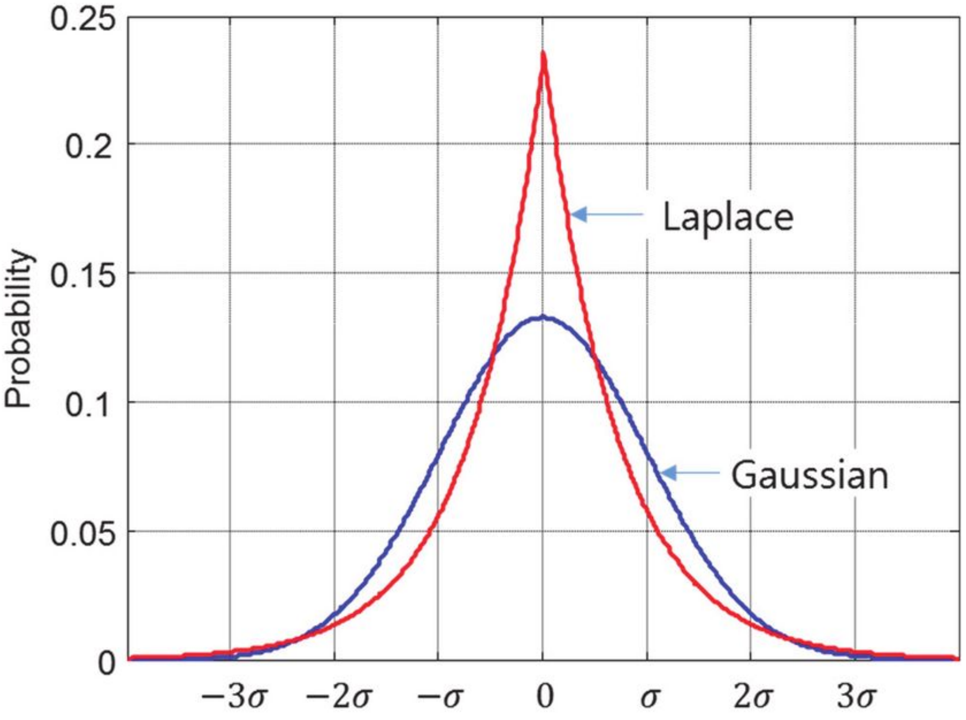

$= L_1$ regularization

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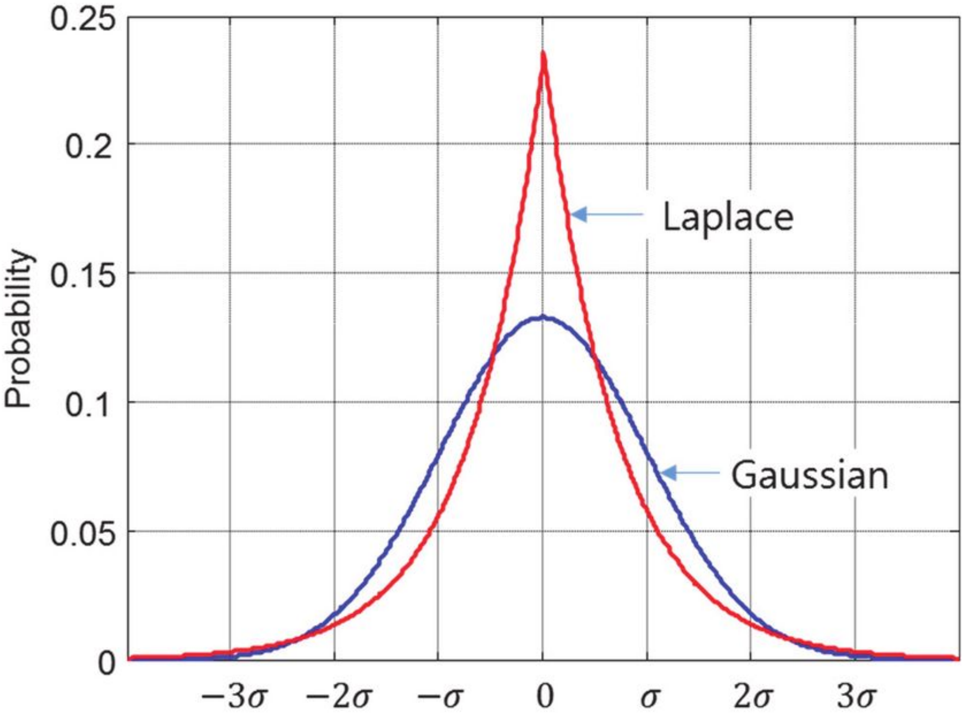

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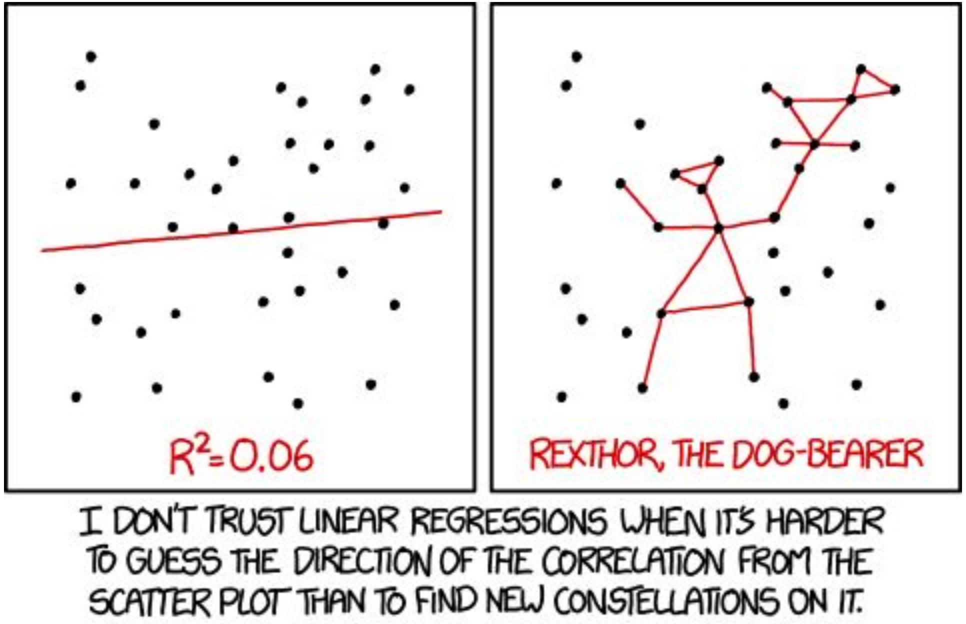
see seminar extra materials for more

Welcome to the church of Bayes

Дмитрий Ветров - заведующий Международной лабораторией глубинного обучения и байесовских методов

That’s all. Practice coming next.


R^2=0.06
REXTHOR, THE DOG-BEARER
I DON'T TRUST LINEAR REGRESSIONS WHEN IT'S HARDER TO GUESS THE DIRECTION OF THE CORRELATION FROM THE SCATTER PLOT THAN TO FIND NEW CONSTELLATIONS ON IT.