# Introduction to Machine Learning

## Gradient and Regularization Methods

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# Outline


1. Linear Regression using Gradient Descent
   - Introduction
   - How do we stabilize the solution?
   - The Basic Algorithm
   - How to obtain $\eta(k)$

2. Regularization Methods
   - Introduction
   - Intuition from Overfitting
   - The Idea of Regularization
   - Ridge Regression
   - The LASSO
     - Lagrange Multipliers
     - The Basic Method
     - The Lagrangian Version of the LASSO
     - Generalization

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**We can develop a more robust algorithm**

- Using the Gradient Descent Idea

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## We can develop a more robust algorithm

- Using the Gradient Descent Idea

## Basically, The Gradient Descent

- It uses the change in the surface of the cost function to obtain a direction of improvement.

# Gradient Descent

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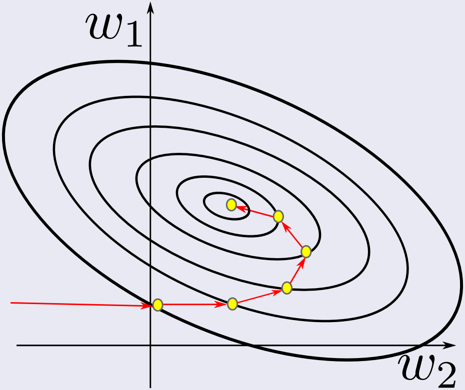
$$\boldsymbol{w}(k+1) = \boldsymbol{w}(k) - \eta(k) \nabla J(\boldsymbol{w}(k)) \quad (1)$$

$\eta(k)$ is a positive scale factor or learning rate!!!

# Geometrically

## We have the following

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# By using a regularized equation

## We have

$$J\left(\boldsymbol{w}\right)=\frac{1}{2}\sum_{i=1}^{N}\left(y_i-\sum_{j=1}^{d+1}x_j^i w_j\right)^2+\frac{\lambda}{2}\sum_{j=1}^{d+1}w_j^2 \tag{2}$$

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## Then, for each $w_j$

$$\frac{dJ(\boldsymbol{w})}{dw_j} = -\sum_{i=1}^{N}\left[\left(y_i - \sum_{j=1}^{d+1} x_j^i w_j\right) x_j^i\right] + \lambda w_j \quad (3)$$

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## Therefore

$$\nabla J\left(\boldsymbol{w}\left(k\right)\right)=\begin{pmatrix}-\sum_{i=1}^{N}\left[\left(y_i-\sum_{j=1}^{d+1}x_j^iw_j\right)x_1^i\right]+\lambda w_1\\ \vdots\\ -\sum_{i=1}^{N}\left[\left(y_i-\sum_{j=1}^{d+1}x_j^iw_j\right)x_{d+1}^i\right]+\lambda w_{d+1}\end{pmatrix}$$

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- If $\eta(k)$ is too small, convergence is quite slow!!!

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- If $\eta(k)$ is too large, correction will overshot and can even diverge!!!

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# Using the Taylor's second-order expansion around value $\boldsymbol{w}(\boldsymbol{k})$

## We do the following

$$J(\boldsymbol{w}) = J(\boldsymbol{w}(k)) + \nabla J^T(\boldsymbol{w} - \boldsymbol{w}(k)) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}(k))^T \boldsymbol{H}(\boldsymbol{w} - \boldsymbol{w}(k)) \quad (4)$$

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## Here, we have

- $\nabla J$ is the vector of partial derivatives $\frac{\partial J}{\partial w_i}$ evaluated at $\boldsymbol{w}\left(k\right)$.

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- $\nabla J$ is the vector of partial derivatives $\frac{\partial J}{\partial w_i}$ evaluated at $\boldsymbol{w}(k)$.
- $\boldsymbol{H}$ is the Hessian matrix of second partial derivatives $\frac{\partial^2 J}{\partial w_i \partial w_j}$ evaluated at $\boldsymbol{w}(k)$.

# Then

**We substitute (Eq. 1) into (Eq. 4)**

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## Finally, we have

$$J(\boldsymbol{w}(k+1)) \cong J(\boldsymbol{w}(k)) - \eta(k) \|\nabla J\|^2 + \frac{1}{2}\eta^2(k) \nabla J^T \boldsymbol{H} \nabla J \tag{6}$$

## Derive with respect to $\eta(k)$ and make the result equal to zero

**We have then**

$$-\|\nabla J\|^2 + \eta(k)\nabla J^T \boldsymbol{H} \nabla J = 0 \tag{7}$$

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## Problem!!!

Calculating $\boldsymbol{H}$ can be quite expansive!!!

# We can have an adaptive linear search!!!

## We can use the idea of having everything fixed, but $\eta\left(k\right)$

Then, we can have the following function
$f\left(\eta\left(k\right)\right) = J\left(\boldsymbol{w}\left(k\right) - \eta\left(k\right)\nabla J\left(\boldsymbol{w}\left(k\right)\right)\right)$

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**Linear Search Methods**

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- Etc.

# Please Take a Look

**For more, please read the paper**

“SEQUENTIAL MINIMAX SEARCH FOR A MAXIMUM” by J. Kiefer

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## Therefore

- Shrinkage methods are more continuous avoiding high variability.

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# The house example

## Imagine the following data set

# Now assume that we use LSE

## For the fitting

$$\frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{w}}\left(x_i\right)-y_i\right)^2$$

# Now assume that we use LSE

## For the fitting

$$\frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{w}}\left(x_i\right)-y_i\right)^2$$

## We can then run one of our machine to see what minimize better the previous equation

Question: Did you notice that I did not impose any structure to $h_{\boldsymbol{w}}\left(x\right)$?

# Then, First fitting

## What about using $h_1(x) = w_0 + w_1 x + w_2 x^2$?

# Second fitting

**What about using $h_2(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$?**

# Therefore, we have a problem

**We get weird overfitting effects!!!**

What do we do? What about minimizing the influence of $w_3, w_4, w_5$?

# Therefore, we have a problem

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What do we do? What about minimizing the influence of $w_3, w_4, w_5$?

## How do we do that?

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left( h_{\boldsymbol{w}} \left( x_i \right) - y_i \right)^2$$

What about integrating those values to the cost function? Ideas

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# We have

**Regularization intuition is as follow**

Small values for parameters $w_0, w_1, w_2, ..., w_n$

# We have

## Regularization intuition is as follow

Small values for parameters $w_0, w_1, w_2, ..., w_n$

## It implies

1. "Simpler" function
2. Less prone to overfitting

# We can do the previous idea for the other parameters

**We can do the same for the other parameters**

$$\min_{\boldsymbol{w}} \frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{w}}\left(x_i\right)-y_i\right)^2+\sum_{i=1}^{d}\lambda_i w_i^2 \tag{9}$$

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## However handling such many parameters can be so difficult

Combinatorial problem in reality!!!

# Better, we can

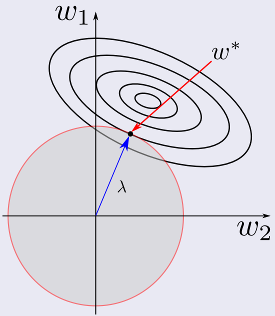
**We better use the following**

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{w}}\left(x_i\right) - y_i\right)^2 + \lambda \sum_{i=1}^{d} w_i^2 \tag{10}$$

# Graphically

## Geometrically Equivalent to

$$\sum_{i=1}^{N}\left(y_i - \boldsymbol{x}_i^T\boldsymbol{w}\right)^2 + \lambda\sum_{i=1}^{d+1} w_i^2$$



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# Ridge Regression

## Equation

$$\widehat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \left\{ \sum_{i=1}^{N} \left( y_i - w_0 - \sum_{j-1}^{d} x_{ij} w_j \right)^2 + \lambda \sum_{j=1}^{d} w_j^2 \right\}$$

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## Here

- $\lambda \geq 0$ is a complexity parameter that controls the amount of shrinkage

# Therefore

**The Larger $\lambda \geq 0$**

- The coefficients are shrunk toward zero (and each other).

# Therefore

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**This is also used in Neural Networks**

- where it is known as weight decay

# This is also can be written

## Optimization Solution

$$\arg\min_{\boldsymbol{w}} \sum_{i=1}^{N} \left( y_i - w_0 - \sum_{j-1}^{d} x_{ij} w_j \right)^2$$

$$\text{subject to } \sum_{j=1}^{d} w_j^2 < t$$

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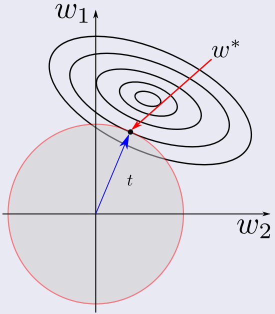
$$\begin{aligned} &\arg\min \ \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}_i^T \boldsymbol{w}\right)^2 \\ &\text{subject to } \sum_{i=1}^{d+1} w_i^2 < t \end{aligned}$$



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# Least Absolute Shrinkage and Selection Operator (LASSO)

**It was introduced by Robert Tibshirani in 1996 based on Leo Breiman's nonnegative garrote**

$$\widehat{\boldsymbol{w}}^{garrote} = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{N} \left( y_i - \beta_0 - \sum_{j=1}^{d} x_{ij} w_j \right)^2 + N\lambda \sum_{j=1}^{d} w_j$$

$$\text{s.t. } w_j > 0 \ \forall j$$

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**Robert Tibshirani proposed the use of the $L_1$ norm**

$$\|\boldsymbol{w}\|_1 = \sum_{i=1}^{d} |w_i|$$

# The Final Optimization Problem

## LASSO

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## This is not derivable

- More advanced methods are necessary to solve this problem!!!

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  - Lagrange Multipliers
  - The Basic Method
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# Lagrange Multipliers

## The method of Lagrange multipliers

- It gives a set of necessary conditions to identify optimal points of equality constrained optimization problems.

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**The method of Lagrange multipliers**

- It gives a set of necessary conditions to identify optimal points of <u>equality constrained</u> optimization problems.

**This is done by converting a constrained problem to an equivalent unconstrained problem**

- with the help of certain unspecified parameters known as <u>Lagrange multipliers</u>.

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## The classical problem formulation

$$\min\ f\left(x_1,...,x_n\right)$$
$$s.t\ h_1\left(x_1,...,x_n\right)=0$$

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$$\min\ \ L\left(x_1, ..., x_n, \lambda\right) = \min\left\{f\left(x_1, ..., x_n\right) - \lambda h_1\left(x_1, ..., x_n\right)\right\}$$

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## where

- $L(\mathbf{x}, \lambda)$ is the Lagrangian function.
- $\lambda$ is an unspecified positive or negative constant called the **Lagrange Multiplier.**

# Finding an Optimum using Lagrange Multipliers

**New problem**

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**New problem**

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**We want a $\lambda = \lambda^*$ optimal**

If the minimum of $L(x_1, ..., x_n, \lambda^*)$ occurs at

$$(x_1, x_2, ..., x_n)^T = (x_1, x_2, ..., x_n)^{T*}$$

# Therefore

**$(x_1, ..., x_n)^{T*}$ satisfies $h_1(x_1, ..., x_n) = 0$, then $(x_1, ..., x_n)^{T*}$ minimizes**

$$\begin{aligned} \min\ & f(x_1, ..., x_n) \\ s.t\ & h_1(x_1, ..., x_n) = 0 \end{aligned}$$

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**Trick**

- It is to find appropriate value for Lagrangian multiplier $\lambda$.

# Remember

**Think about this**

Remember First Law of Newton!!!

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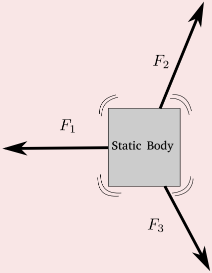
## Yes!!!

**A system in equilibrium does not move**



# Lagrange Multipliers

**Definition**

Gives a set of necessary conditions to identify optimal points of equality constrained optimization problem

# Lagrange was a Physicists

## He was thinking in the following formula

A system in equilibrium has the following equation:

$$F_1 + F_2 + ... + F_K = 0 \tag{11}$$

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## Think about the following

The Gradient of a surface.

# Gradient to a Surface

**After all a gradient is a measure of the maximal change**

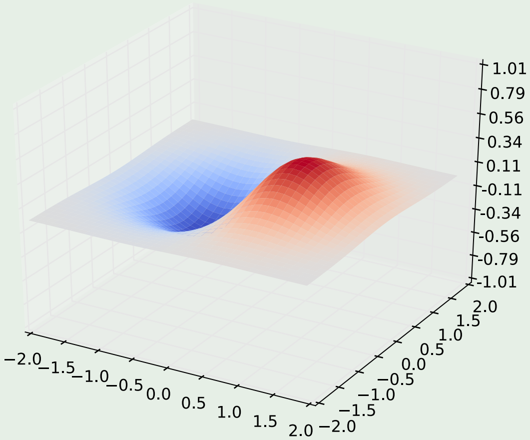
For example the gradient of a function of three variables:

$$\nabla f(\boldsymbol{x}) = i\frac{\partial f(\boldsymbol{x})}{\partial x} + j\frac{\partial f(\boldsymbol{x})}{\partial y} + k\frac{\partial f(\boldsymbol{x})}{\partial z} \tag{12}$$

where $i$, $j$ and $k$ are unitary vectors in the directions $x$, $y$ and $z$.

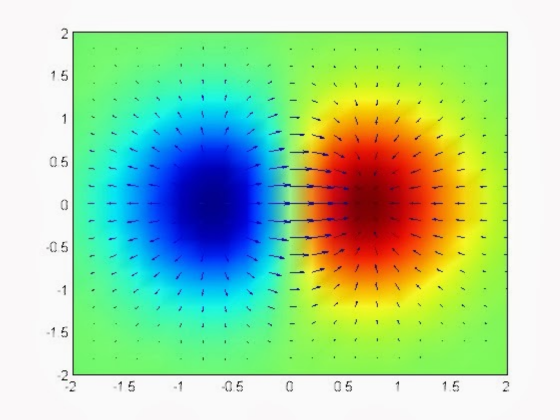
# Example

## We have $f(x, y) = x \exp\{-x^2 - y^2\}$



# Example

## With Gradient at the the contours when projecting in the 2D plane

100 

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**Yes, we can use the gradient**

However, we need to do some scaling of the forces by using parameters $\lambda$

# Now, Think about this

**Yes, we can use the gradient**

However, we need to do some scaling of the forces by using parameters $\lambda$

**Thus, we have**

$$F_0 + \lambda_1 F_1 + ... + \lambda_K F_K = 0 \tag{13}$$

where $F_0$ is the gradient of the principal cost function and $F_i$ for $i = 1, 2, .., K$.

## Thus

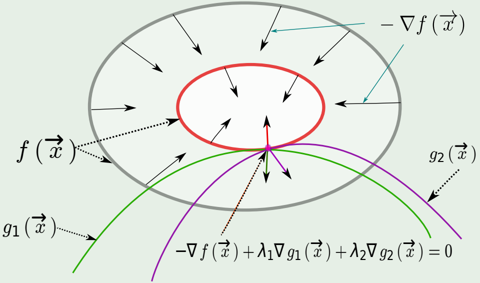
If we have the following optimization:

$$
\begin{aligned}
\min \;\; & f(\boldsymbol{x}) \\
s.t g_1(\boldsymbol{x}) &= 0 \\
g_2(\boldsymbol{x}) &= 0
\end{aligned}
$$

# Geometric interpretation in the case of minimization

**What is wrong? Gradients are going in the other direction, we can fix by simple multiplying by -1**

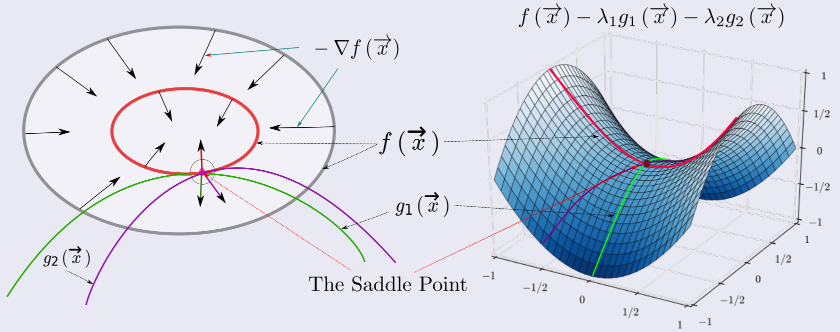
Here the cost function is $f(x,y) = x\exp\left\{-x^2 - y^2\right\}$ we want to minimize




Nevertheless: it is equivalent to $\nabla f(\vec{x}) - \lambda_1 \nabla g_1(\vec{x}) - \lambda_2 \nabla g_2(\vec{x}) = 0$

# Basically, we convert the problem into a one looking for a **Saddle Point**

## At the left the original problem, at the right the Lagrangian!!!



# Yes!!!

## Basically

- We convert the minimization or maximization of a convex or concave section of a function living in a constrained environment!!!

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$$\sum_{i=1}^{N} \left(y_i - \boldsymbol{x}^T \boldsymbol{w}\right)^2 + \lambda \sum_{i=1}^{d} |w_i| \tag{14}$$

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## From the step 2

If there are $n$ variables (i.e., $x_1, \cdots, x_n$) then you will get $n$ equations with $n + 1$ unknowns (i.e., $n$ variables $x_i$ and one Lagrangian multiplier $\lambda$).

# Example

**We can apply that to the following problem**

$$\min \ f(x,y) = x^2 - 8x + y^2 - 12y + 48$$
$$s.t \ x + y = 8$$

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# The Lagrangian Version

## The Lagrangian

$$\widehat{\boldsymbol{w}}^{LASSO} = \arg\min_{\boldsymbol{w}} \left\{ \sum_{i=1}^{N} \left( y_i - \boldsymbol{x}^T \boldsymbol{w} \right)^2 + \lambda \sum_{i=1}^{d} |w_i| \right\}$$

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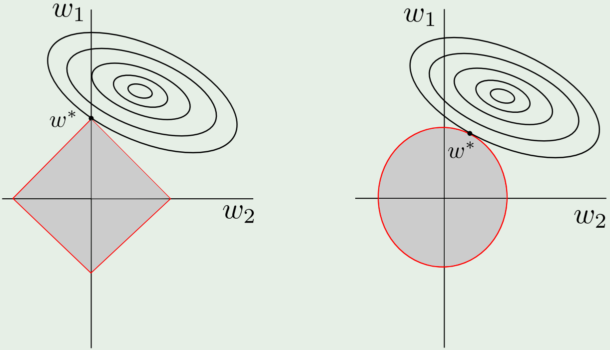
## However

- You have other regularizations as $\|\boldsymbol{w}\|_2 = \sqrt{\sum_{i=1}^{d} |w_i|^2}$

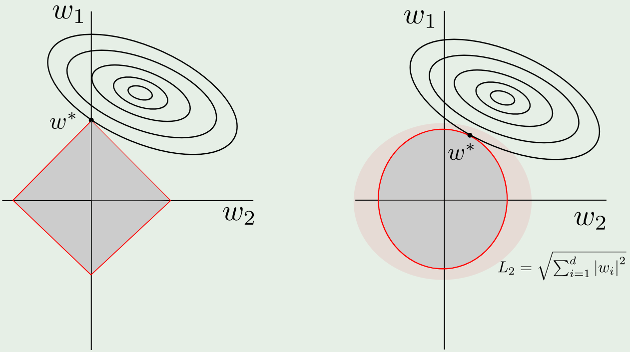
# Graphically

**The first area correspond to the $L_1$ regularization and the second one?**



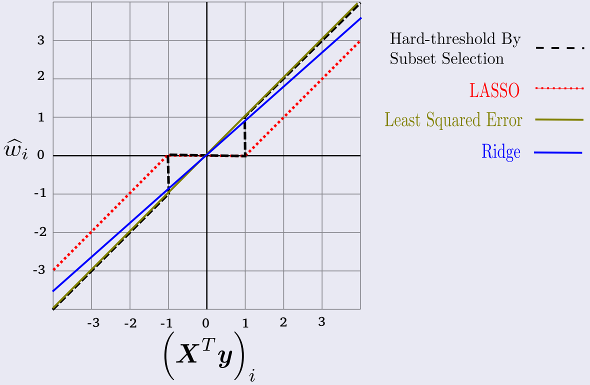
# Graphically

**Yes the circle defined as $\|\boldsymbol{w}\|_2 = \sqrt{\sum_{i=1}^{d} |w_i|^2}$**



# For Example

## In the Case of $\boldsymbol{X}$ is a Orthogonal Matrix



# The seminal paper by Robert Tibshirani

**An initial study of this regularization can be seen in**

"Regression Shrinkage and Selection via the LASSO" by Robert Tibshirani - 1996

# This out the scope of this class

**However, it is worth noticing that the most efficient method for solving LASSO problems is**

"Pathwise Coordinate Optimization" By Jerome Friedman, Trevor Hastie, Holger Ho and Robert Tibshirani

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**Nevertheless**

It will be a great seminar paper!!!

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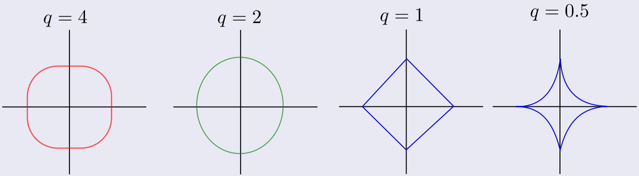
# Furthermore

**We can generalize ridge regression and the lasso, and view them as Bayes estimates**

$$\widehat{\boldsymbol{w}}^{LASSO} = \arg\min_{\boldsymbol{w}} \left\{ \sum_{i=1}^{N} \left( y_i - \boldsymbol{x}^T \boldsymbol{w} \right)^2 + \lambda \sum_{i=1}^{d} |w_i|^q \right\} \text{ with } q \geq 0$$

# For Example

## We have when $d = 2$



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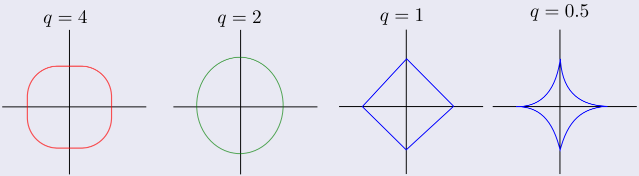


## Here, when $q > 1$

- You are having a derivable Lagrangian, but you lose the LASSO properties

# Therefore

**Zou and Hastie (2005) introduced the elastic- net penalty**

$$\lambda \sum_{i=1}^{d} \left\{ \alpha w_i^2 + (1-\alpha)\,|w_i| \right\}$$

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**This is Basically**

- A Compromise Between the Ridge and LASSO.