Introduction to Machine Learning

Gradient and Regularization Methods

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Outline

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Given that the Canonical Solution has problems

We can develop a more robust algorithm

- Using the Gradient Descent Idea

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- 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.

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The basic procedure is as follow

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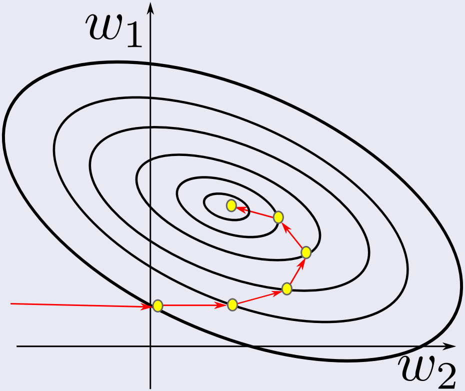
$\eta(k)$ is a positive scale factor or learning rate!!!

Geometrically

We have the following



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For our full regularized equation

We have

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

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Then, for each w_j

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

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Therefore

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

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

Outline

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

We do the following

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

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Remark: This is know as Taylor's Second Order expansion!!!

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- ∇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

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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 $\eta(k)$

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

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Linear Search Methods

- Backtracking linear search
- Bisection method
- Golden ratio
- Etc.

Please Take a Look

For more, please read the paper

"SEQUENTIAL MINIMAX SEARCH FOR A MAXIMUM" by J. Kiefer

There are better versions

Take a look

The papers at the repository.

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Shrinkage Methods

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However given process

- it often exhibits high variance,
- It does not reduce the prediction error of the full model.

Therefore

- Shrinkage methods are more continuous avoiding high variability.

Outline

The house example

Imagine the following data set

Now assume that we use LSE

For the fitting

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

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

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?

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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

Outline

We have

Regularization intuition is as follow

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

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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

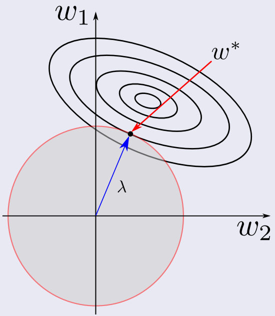
We better use the following

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

Graphically

Geometrically Equivalent to

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



Outline

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 $\lambda \geq 0$

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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

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

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

Graphically

Geometrically Equivalent to

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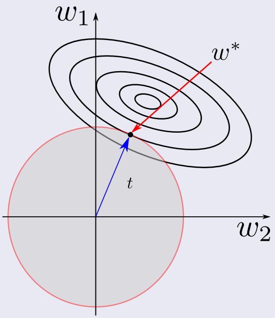

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Here, we have problem

We have pointed out that all the features are treated equally

- At Least Squared Error Cost function

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Therefore, we need to do to obtain

- Good features to this type of classifiers

Principal Component Analysis A.K.A. Karhunen-Loeve Transform

Setup

- Consider a data set of observations $\{\boldsymbol{x}_n\}$ with $n = 1, 2, ..., N$ and $\boldsymbol{x_n} \in R^d$.

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Goal

Project data onto space with dimensionality $m < d$ (We assume m is given)

Dimensional Variance

Remember the Variance Sample

$$VAR(X) = \frac{\sum_{i=1}^{N} (x_i - \overline{x})(x_i - \overline{x})}{N-1} \tag{11}$$

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You can do the same in the case of two variables X and Y

$$COV(X,Y) = \frac{\sum_{i=1}^{N} (x_i - \overline{x})(y_i - \overline{y})}{N-1} \tag{12}$$

Now, Define

Given the data

$$\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_N \tag{13}$$

where $\boldsymbol{x}_i$ is a column vector

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Build new data

$$\boldsymbol{x}_1 - \overline{\boldsymbol{x}}, \boldsymbol{x}_2 - \overline{\boldsymbol{x}}, ..., \boldsymbol{x}_N - \overline{\boldsymbol{x}} \tag{15}$$

Build the Sample Mean

The Covariance Matrix

$$S = \frac{1}{N-1} \sum_{i=1}^{N} \left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)^T \tag{16}$$

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Properties

1. The ijth value of S is equivalent to σ_{ij}^2.
2. The iith value of S is equivalent to σ_{ii}^2.
3. What else? Look at a plane Center and Rotating!!!

Using S to Project Data

As in Fisher

We want to project the data to a line...

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Question

What is the Sample Variance of the Projected Data

Thus we have

Variance of the projected data

$$\frac{1}{N-1}\sum_{i=1}^{N}\left[\boldsymbol{u}_1\boldsymbol{x}_i - \boldsymbol{u}_1\overline{\boldsymbol{x}}\right]\left[\boldsymbol{u}_1\boldsymbol{x}_i - \boldsymbol{u}_1\overline{\boldsymbol{x}}\right]^T = \boldsymbol{u}_1^T S \boldsymbol{u}_1 \tag{17}$$

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Use Lagrange Multipliers to Maximize

$$\boldsymbol{u}_1^T S\boldsymbol{u}_1 + \lambda_1\left(1 - \boldsymbol{u}_1^T\boldsymbol{u}_1\right) \tag{18}$$

Derive by $\boldsymbol{u}_1$

We get

$$S\boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1 \tag{19}$$

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Then

$\boldsymbol{u}_1$ is an eigenvector of S.

If we left-multiply by $\boldsymbol{u}_1$

$$\boldsymbol{u}_1^T S \boldsymbol{u}_1 = \lambda_1 \tag{20}$$

Thus

Variance will be the maximum when

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is set to the largest eigenvalue. Also know as the First Principal Component

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By Induction

It is possible for M-dimensional space to define M eigenvectors $\boldsymbol{u}_1, \boldsymbol{u}_2, ..., \boldsymbol{u}_M$ of the data covariance S corresponding to $\lambda_1, \lambda_2, ..., \lambda_M$ that maximize the variance of the projected data.

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Computational Cost

1. Full eigenvector decomposition $O\left(d^3\right)$
2. Power Method $O\left(Md^2\right)$ "Golub and Van Loan, 1996)"
3. Use the Expectation Maximization Algorithm

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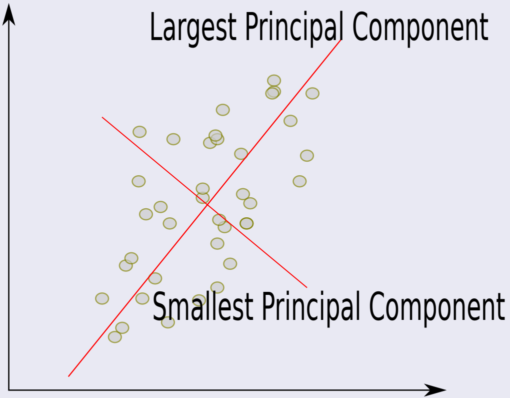

Example

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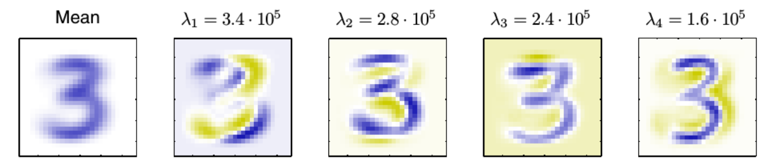

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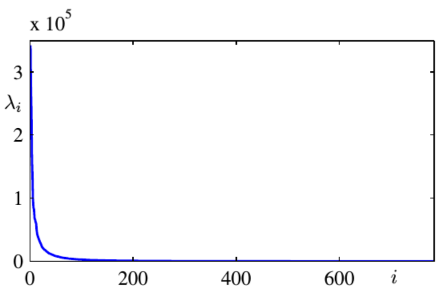
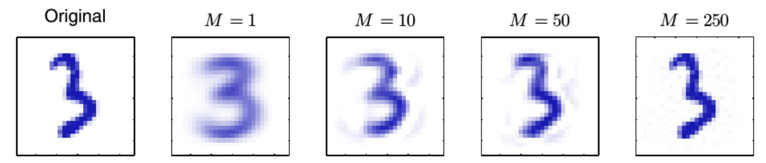


Example

From Bishop



Outline

Least Absolute Shrinkage and Selection Operator (LASSO)

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

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

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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

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

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This is not derivable

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

Outline

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

- with the help of certain unspecified parameters known as Lagrange multipliers.

Lagrange Multipliers

The classical problem formulation

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

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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.
- λ is an unspecified positive or negative constant called the **Lagrange Multiplier.**

Finding an Optimum using Lagrange Multipliers

New problem

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Finding an Optimum using Lagrange Multipliers

New problem

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

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

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Trick

- It is to find appropriate value for Lagrangian multiplier λ.

Remember

Think about this

Remember First Law of Newton!!!

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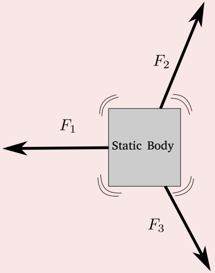
Yes!!!

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:

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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

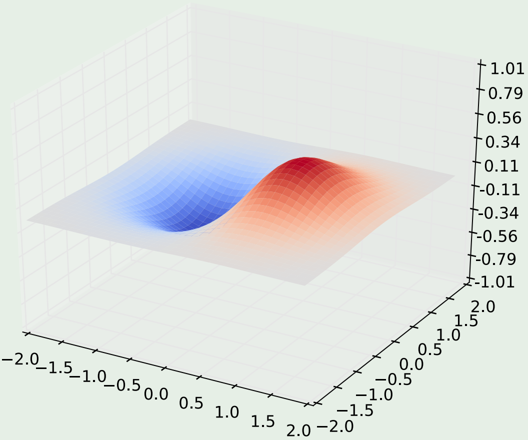
For example the gradient of a function of three variables:

$$\nabla f(\boldsymbol{x}) = i\frac{\partial f(\boldsymbol{x})}{\partial x} + j\frac{\partial f(\boldsymbol{x})}{\partial y} + k\frac{\partial f(\boldsymbol{x})}{\partial z} \tag{23}$$

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

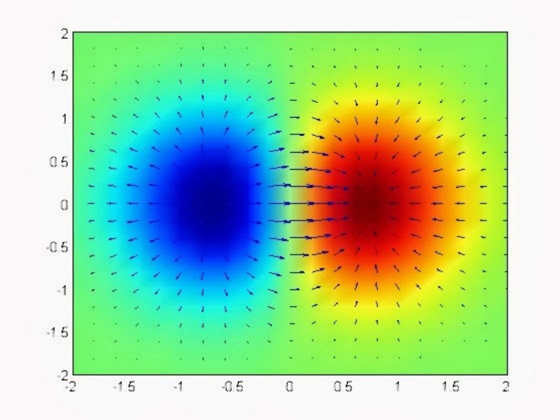
Example

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



Example

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



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Now, Think about this

Yes, we can use the gradient

However, we need to do some scaling of the forces by using parameters λ

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Yes, we can use the gradient

However, we need to do some scaling of the forces by using parameters λ

Thus, we have

$$F_0 + \lambda_1 F_1 + ... + \lambda_K F_K = 0 \tag{24}$$

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

Thus

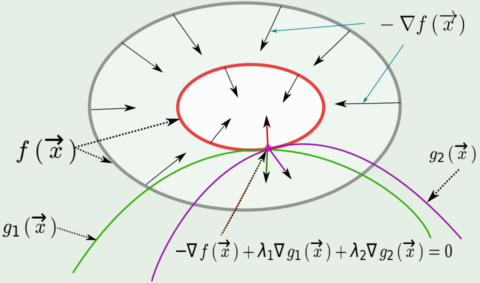
If we have the following optimization:

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

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

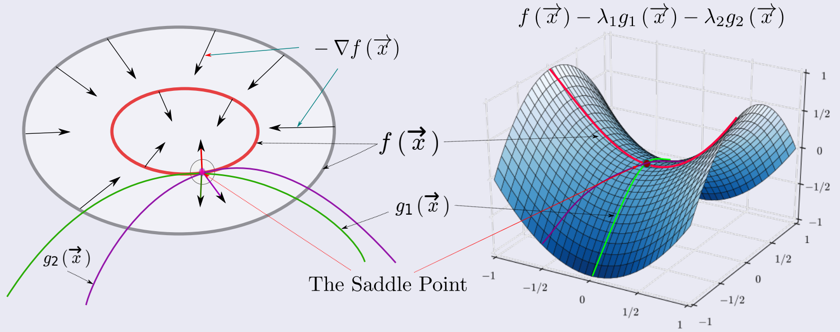
Here the cost function is $f(x, y) = x \exp\{-x^2 - y^2\}$ we want to minimize



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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Method

Steps

1. Original problem is rewritten as:
   1. minimize $L(\boldsymbol{x}, \lambda) = f(\boldsymbol{x}) - \lambda h_1(\boldsymbol{x})$

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$$\sum_{i=1}^{N} \left(y_i - \boldsymbol{x}^T \boldsymbol{w}\right)^2 + \lambda \sum_{i=1}^{d} |w_i| \tag{25}$$

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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 λ).

Example

We can apply that to the following problem

$$
\begin{aligned}
\min \; & f(x,y) = x^2 - 8x + y^2 - 12y + 48 \\
s.t \; & x + y = 8
\end{aligned}
$$

Outline

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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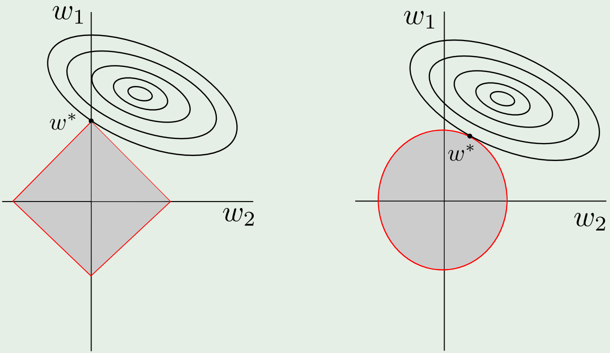
However

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

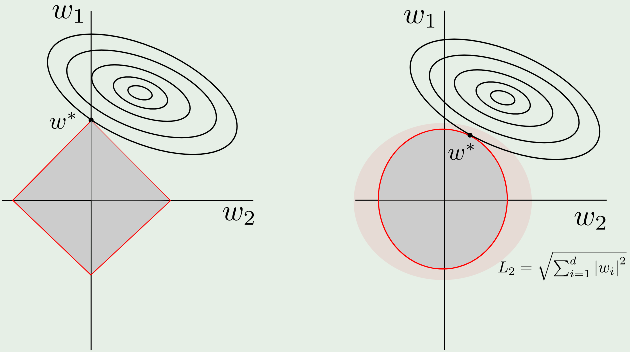
Graphically

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



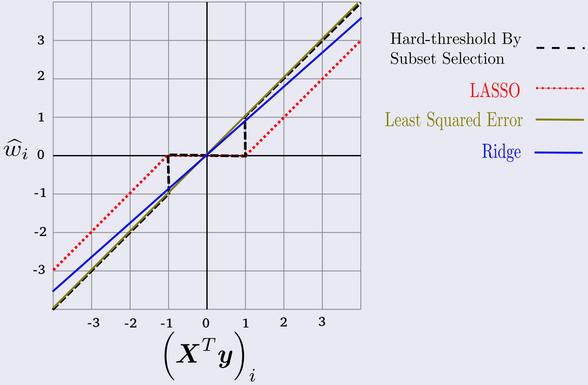
Graphically

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

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Nevertheless

It will be a great seminar paper!!!

Outline

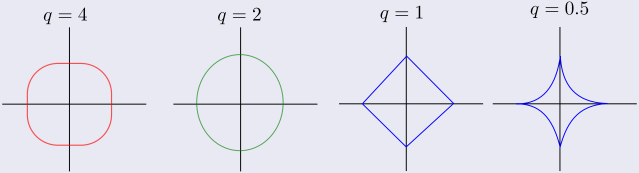
Furthermore

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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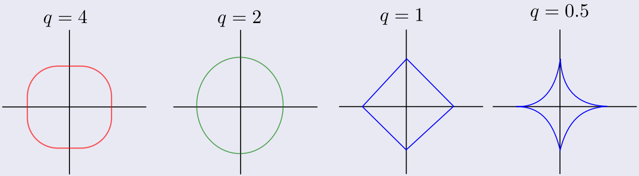

Here, when $q > 1$

- 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.