CS 236756 - Technion - Intro to Machine Learning

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Tutorial 07 - Optimization

Agenda

In [1]:
```
# imports for the tutorial
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
%matplotlib notebook
```

Optimization Problems

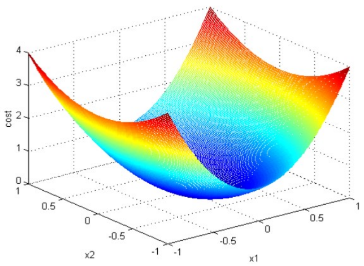
Definitions

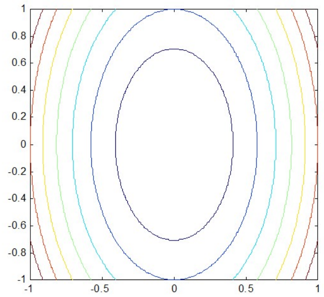
- **Objective Function** - mathematical function which is optimized by changing the values of the design variables.
- **Design Variables** - variables that we, as designers, can change.
- **Constraints** - functions of the design variables which establish limits in individual variables or combinations of design.
    - For example - "Find θ that minimizes $f_\theta(x)$ s.t. (subject to) $\theta \leq 1$"

The main problem in optimization is *how* to search for the values of decision variables that minimize the cost/objective function.

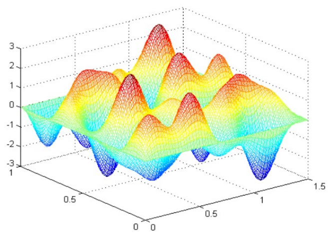
Types of Objective Functions

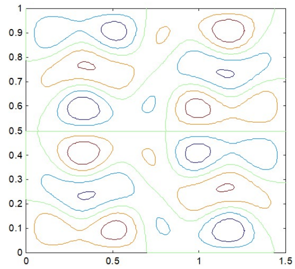
- **Unimodal** - only **one** optimum, that is, the *local* optimum is also global.





- **Multimodal** - more than one optimum





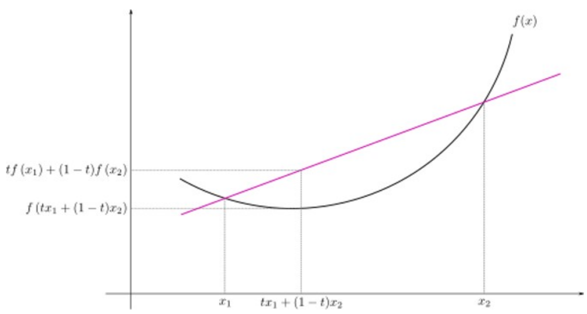
Most search schemes are based on the assumption of **unimodal** surface. The optimum determined in such cases is called **local optimum design**.

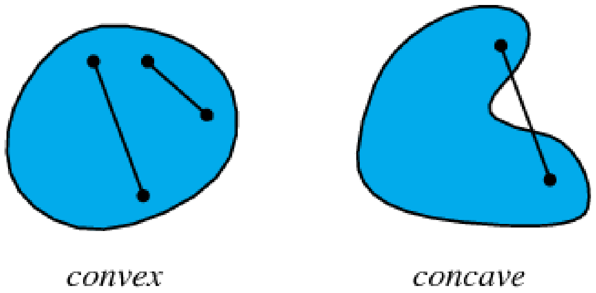
The **global optimum** is the best of all *local optimum* designs.

Convexity

- **Definition**:

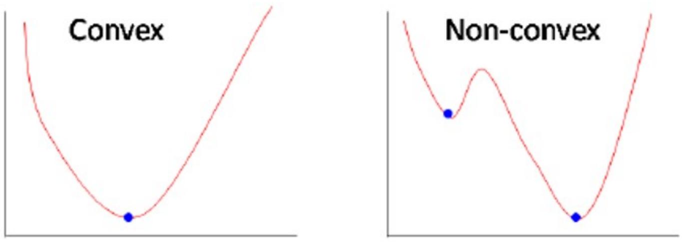
$$\forall x_1, x_2 \in X, \forall t \in [0,1] :$$
$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$





[Image Source (http://mathworld.wolfram.com/Convex.html)](http://mathworld.wolfram.com/Convex.html)

- Convex functions are **unimodal**



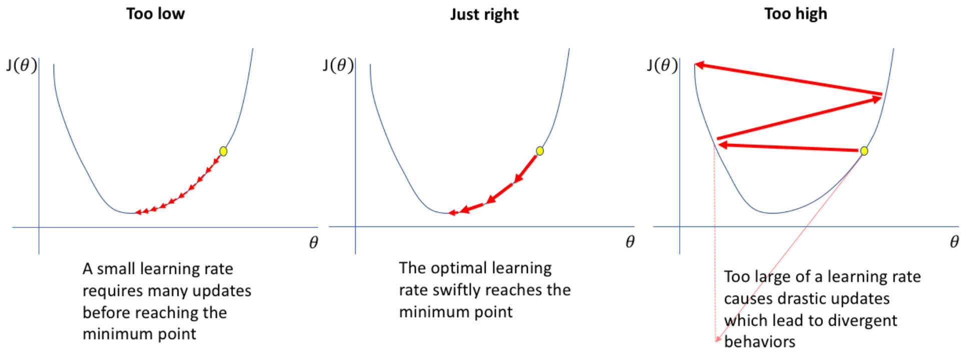
Continuous Optimization

- Derivative based optimization - the search directions are determined based on deivative information
- Methods include:
  - **Gradient Descent**
  - Newton method
  - Conjugate gradient
- We will focus on *Gradient Descent*

1-D Optimization

(Batch) Gradient Descent

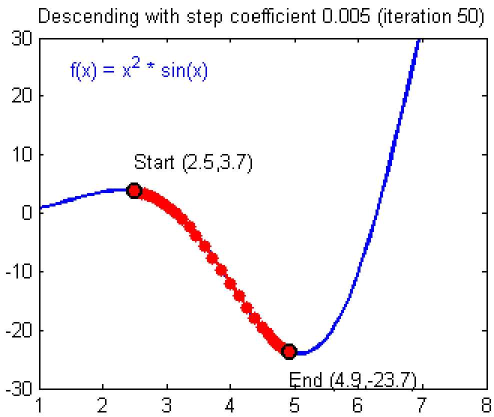
- Generic optimization algorithm capable of finding optimal solutions to a wide range of problems.
- The general idea is to tweak parameters **iteratively** to minimize a cost function.
- It measures the local gradient of the error function with regards to the parameter vector (θ or w), and it goes down in the direction of the descending gradient. Once the gradient is zero - the minimum is reached (=convergence).

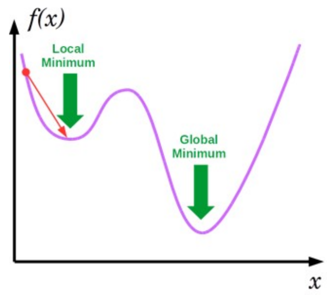
- **Learning Rate** hyperparameter - it is the size of step to be taken in each iteration.
  - Too *small* $\rightarrow$ the algorithm will have to go through many iterations to converge, which will take a long time
  - Too *high* $\rightarrow$ might make the algorithm diverge as it may miss the minimum
  - 

    [Image Source (https://www.jeremyjordan.me/nn-learning-rate/)](https://www.jeremyjordan.me/nn-learning-rate/)

- **Pseudocode**:
  - **Require**: Learning rate α_k
  - **Require**: Initial parameter w
  - **While** stopping criterion not met **do**
    - Compute gradient: $g \leftarrow f'(x, w)$ (more specifically, for M samples: $g \leftarrow \frac{1}{M}\sum_{i=1}^{M} f'(x_i, w)$, where f' is w.r.t θ or w)
    - Apply update: $w \leftarrow w - \alpha_k g$
    - $k \leftarrow k + 1$
  - **end while**

- **Visualization**:





- **Convergene**: When the cost function is *convex* and its slope does not change abruptly, (Batch) GD with a *fixed* learning rate will eventually converge to the optimal solution (but the time is depndent on the rate).

Example - Linear Least Squares

- **Problem Formulation**
  - $y \in \mathbb{R}^N$ - vector of values
  - $X \in \mathbb{R}^N$ - data matrix with *one feature* (= data *vector*)
  - $w \in \mathbb{R}$ - the *parameter* to be learnt
- **Goal**: find w that best fits the measurement y
- Mathematically:

$$\min_w f(w; x, y) = \min_w \sum_{i=1}^{N} (wx_i - y_i)^2$$

- In vector form:

$$\min_w f(w; x, y) = \min_w ||wX - Y||_2^2$$

LLS - Analytical Solution

- Mathematically:

$$\min_w f(w; x, y) = \min_w \sum_{i=1}^{N} (wx_i - y_i)^2 = \min_w \sum_{i=1}^{N} w^2x_i^2 - 2wx_iy_i + y_i^2$$

- The derivative:

$$\sum_{i=1}^{N} 2wx_i^2 - 2x_iy_i = 0 \rightarrow w = \frac{\sum_{i=1}^{N} y_i x_i}{\sum_{i=1}^{N} x_i^2}$$

- The second derivative, to ensure minimum:

$$f''(w; x, y) = \sum_{i=1}^{N} 2x_i^2 > 0 \rightarrow good!$$

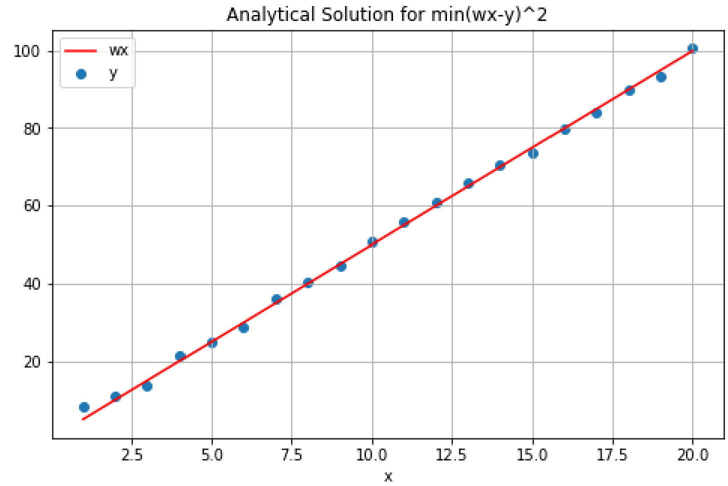
In [2]:
```
# generate some random data
N = 20
x = np.linspace(1, 20, N)
y = 5 * x + np.random.randn(N)
```

In [3]:
```
# lls - analytical solution
# we want to find w that minimizes (wx-y)^2
# by the above derivation
w = np.sum(y * x) / np.sum(np.square(x))
print("best w:", w)
```

```
best w: 4.991854494561919
```

In [6]:
```
def plot_lls_sol(x, y, w, title=""):
    fig = plt.figure(figsize=(8,5))
    ax = fig.add_subplot(1,1,1)
    ax.scatter(x, y, label="y")
    ax.plot(x, w * x, label="wx", color='r')
    ax.legend()
    ax.grid()
    ax.set_xlabel("x")
    ax.set_title(title)
```

In [7]:
```
# let's plot
plot_lls_sol(x, y, w, "Analytical Solution for min(wx-y)^2")
```



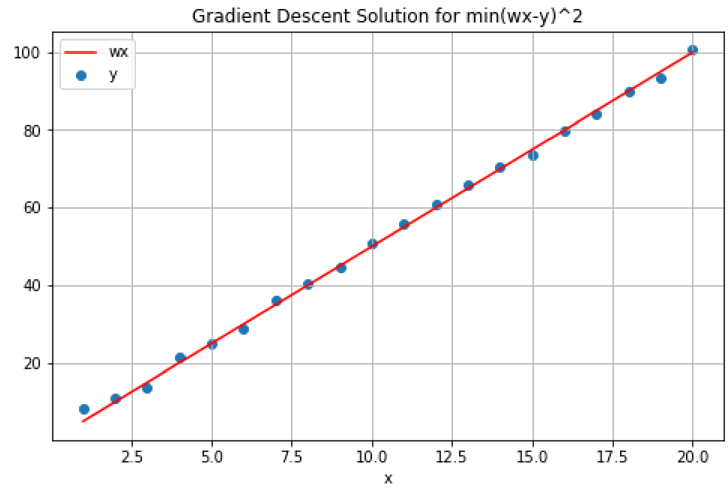
LLS - Gradient Descent Solution

- **Pseudocode**:
  - **Require**: Learning rate α_k
  - **Require**: Initial parameter w
  - **While** stopping criterion not met **do**
    - Compute gradient: $g \leftarrow \frac{1}{N}\sum_{i=1}^{N} 2wx_i^2 - 2x_iy_i$
    - Apply update: $w \leftarrow w - \alpha_k g$
    - $k \leftarrow k + 1$
  - **end while**

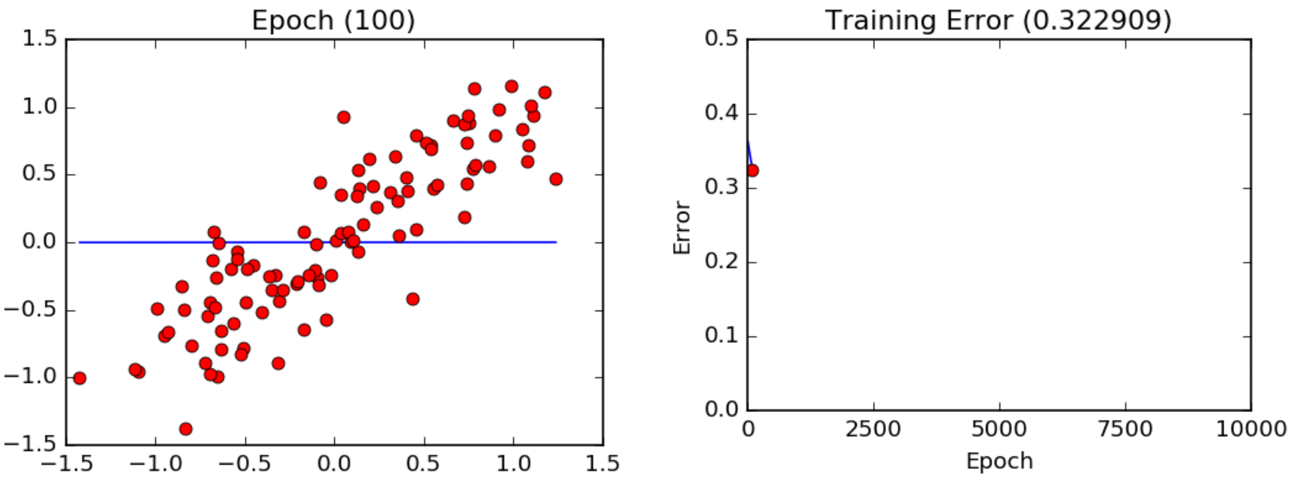
In [8]:
```python
# lls - gradient descent solution
N = 20 # num samples
num_iterations = 20
alpha_k = 0.005
# we want to find w that minimizes (wx-y)^2
# initialize w
w = 0
for i in range(num_iterations):
    print("iter:", i, " w = ", w)
    gradient = np.sum(2 * w * np.square(x) - 2 * x * y) / N
    w = w - alpha_k * gradient
print("best w:", w)
```

```
iter: 0  w =  0
iter: 1  w =  7.163311199696355
iter: 2  w =  4.04727082782844
iter: 3  w =  5.4027483895909825
iter: 4  w =  4.813115650224277
iter: 5  w =  5.069605891848794
iter: 6  w =  4.9580326367421295
iter: 7  w =  5.0065670027135285
iter: 8  w =  4.98545455351597
iter: 9  w =  4.994638468916908
iter: 10  w =  4.9906434657175
iter: 11  w =  4.9923812921092425
iter: 12  w =  4.991625337628834
iter: 13  w =  4.991954177827812
iter: 14  w =  4.991811132341256
iter: 15  w =  4.991873357127908
iter: 16  w =  4.991846289345715
iter: 17  w =  4.991858063830969
iter: 18  w =  4.991852941929883
iter: 19  w =  4.991855169956855
best w: 4.991854200765123
```

In [9]:
```python
plot_lls_sol(x, y, w, "Gradient Descent Solution for min(wx-y)^2")
```



- **Least Squares Visualization**:

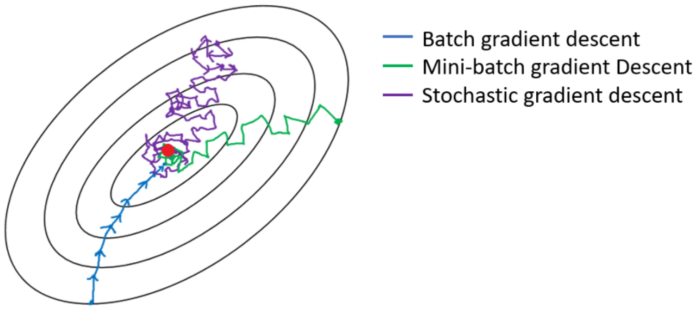


Stochastic Gradient Descent (Mini-Batch Gradient Descent)

- The main problem with (Batch) GD is that it uses the **whole** training set to compute the gradients. But what if that training set is huge? Computing the gradient can take a very long time.
- *Stochastic* Gradient Descent on the other hand, samples just one instance randomly at every step and computes the gradients based on that single instance. This makes the algorithm much faster but due to its randomness, it is much less stable. Instead of steady decreasing untill reaching the minimum, the cost function will bounce up and down, **decreasing only on average**. With time, it will get *very close* to the minimum, but once it is there it will continue to bounce around!
- The final parameters are good but **not optimal**.

- When the cost function is very irregular, this bouncing can actually help the algorithm escape local minima, so SGD has better chance to find the *global* minimum.
- How to find optimal parameters using SGD?
  - **Reduce the learning rate gradually**: this is called *learning schedule*
    - But don't reduce too quickly or you will get stuck at a local minimum or even frozen!
- *Mini-Batch* Gradient Descent - same idea as SGD, but instead of one instance each step, m samples.
  - Get a little bit closer to the minimum than SGD but a little harder to escape local minima.

- **Pseudocode**:
  - **Require**: Learning rate α_k
  - **Require**: Initial parameter w
  - **While** stopping criterion not met **do**
    - Sample a minibatch of m examples from the training set ($m = 1$ for SGD)
    - Set $\{x_1, \dots, x_m,\}$ with corresponding targets $\{y_1, \dots, y_m\}$
    - Compute gradient: $g \leftarrow \frac{1}{m} \sum_{i=1}^{m} f'(x_i, w)$
    - Apply update: $w \leftarrow w - \alpha_k g$
    - $k \leftarrow k + 1$
  - **end while**



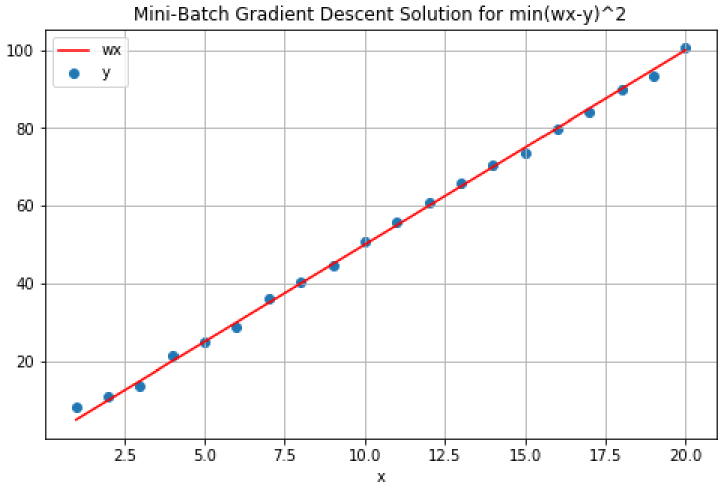
[Image Source (https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3)](https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3)

In [10]:
```python
def batch_generator(x, y, batch_size, shuffle=True):
    """
    This function generates batches for a given dataset x.
    """
    N = len(x)
    num_batches = N // batch_size
    batch_x = []
    batch_y = []
    if shuffle:
        # shuffle
        rand_gen = np.random.RandomState(0)
        shuffled_indices = rand_gen.permutation(np.arange(len(x)))
        x = x[shuffled_indices]
        y = y[shuffled_indices]
    for i in range(N):
        batch_x.append(x[i])
        batch_y.append(y[i])
        if len(batch_x) == batch_size:
            yield np.array(batch_x), np.array(batch_y)
            batch_x = []
            batch_y = []
    if batch_x:
        yield np.array(batch_x), np.array(batch_y)
```

In [11]:
```
# mini-batch gradient descent
batch_size = 5
num_batches = N // batch_size
print("total batches:", num_batches)
num_iterations = 20
alpha_k = 0.001
batch_gen = batch_generator(x, y, batch_size, shuffle=True)
# we want to find w that minimizes (wx-y)^2
# initialize w
w = 0
for i in range(num_iterations):
    for batch_i, batch in enumerate(batch_gen):
        batch_x, batch_y = batch
        if batch_i % 5 == 0:
            print("iter:", i, "batch:", batch_i, " w = ", w)
        gradient = np.sum(2 * w * np.square(batch_x) - 2 * batch_x * batch_y) / len(batch_x)
        w = w - alpha_k * gradient
    batch_gen = batch_generator(x, y, batch_size, shuffle=True)
print("best w:", w)
```

```
total batches: 4
iter: 0 batch: 0  w =  0
iter: 1 batch: 0  w =  3.7248360403288565
iter: 2 batch: 0  w =  4.672774185727788
iter: 3 batch: 0  w =  4.9140161404805225
iter: 4 batch: 0  w =  4.9754101048603685
iter: 5 batch: 0  w =  4.991034331028397
iter: 6 batch: 0  w =  4.99501055973126
iter: 7 batch: 0  w =  4.996022475107257
iter: 8 batch: 0  w =  4.996279998706801
iter: 9 batch: 0  w =  4.996345536207166
iter: 10 batch: 0  w =  4.996362214926948
iter: 11 batch: 0  w =  4.9963664595150385
iter: 12 batch: 0  w =  4.9963675397255285
iter: 13 batch: 0  w =  4.996367814629636
iter: 14 batch: 0  w =  4.996367884590323
iter: 15 batch: 0  w =  4.996367902394706
iter: 16 batch: 0  w =  4.996367906925765
iter: 17 batch: 0  w =  4.99636790807888
iter: 18 batch: 0  w =  4.996367908372338
iter: 19 batch: 0  w =  4.99636790844702
best w: 4.996367908466026
```

In [12]:
```
# let's plot
plot_lls_sol(x, y, w, "Mini-Batch Gradient Descent Solution for min(wx-y)^2")
```



GD Comparison Summary

Method	Accuracy	Update Speed	Memory Usage	Online Learning
Batch Gradient Descent	Good	Slow	High	No
Stochastic Gradient Descent	Good (with softening)	Fast	Low	Yes
Mini-Batch Gradient Descent	Good	Medium	Medium	Yes (depends on the MB size)

- **"Online"** - samples arrive while the algorithm runs (that is, when the algorithm starts running, not all samples exist)
- Note: All of the Gradient Descent algorithms require **scaling** if the feaures are not within the same range!

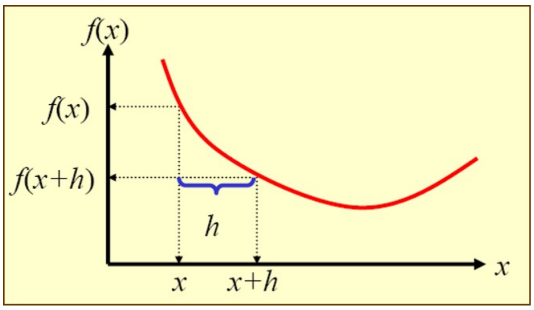
Challenges

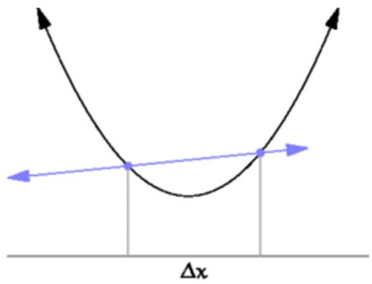
- Choosing a **learning rate**
  - Defining **learning schedule**
- Working with features of different scales (e.g. heights (cm), weights (kg) and age (scalar))
- Avoiding **local minima** (or *suboptimal* minima)

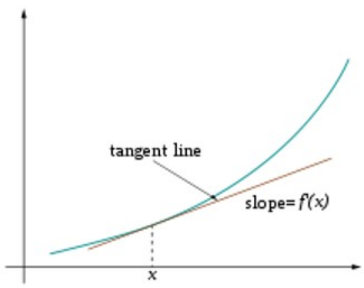
Mathematical Background

Multivariate Calculus

- **The Derivative** - the derivative of $f: \mathbb{R} \to \mathbb{R}$ is a *function* $f': \mathbb{R} \to \mathbb{R}$ given by:
$$f'(x) = \frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$
  - Illustration:

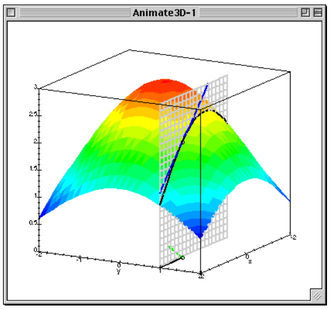




- Rewrite the above:
$$\lim_{h \to 0} \frac{f(x+h) - f(x) - f'(x) \cdot h}{h} = 0$$
  - 

- **The Gradient** - the gradient of $f : \mathbb{R}^N \to \mathbb{R}$ is a *function* $\nabla f : \mathbb{R}^N \to \mathbb{R}^N$ given by:

$$\lim_{h \to 0} \frac{||f(\overline{x} + \overline{h}) - f(\overline{x}) - \nabla f(\overline{x}) \cdot \overline{h}||}{||\overline{h}||} = 0$$

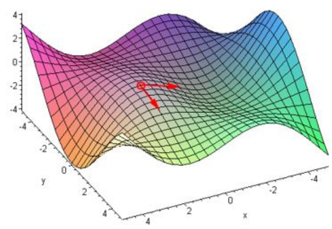
  - 

- The gradient can be expressed in terms of the function's **partial derivatives**:

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

  - Illustration:

$$\nabla f(x) \triangleq \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$



- **The Hessian Matrix**
  - Definition: $H(f)(x)_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(x)$
  -

$$\begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Matrix Calculus - Vector & Matrix Derivatives

- We will use most of the derivations "as is" without derivation.
- A good reference: [The Matrix Cookbook (http://www2.imm.dtu.dk/pubdb/views/edoc_download.php/3274/pdf/imm3274.pdf)](http://www2.imm.dtu.dk/pubdb/views/edoc_download.php/3274/pdf/imm3274.pdf)
- ⚠ **REMEMBER** - ALWAYS write the dimensions of each component and identify whether the expression is a **matrix, vector or scalar**!

Derivative of Vector Multiplication

- Let $x, a \in \mathbb{R}^N \rightarrow x, a$ are vectors
- $\frac{\partial x^T a}{\partial x} = \frac{\partial a^T x}{\partial x} = a$
  - $x^T a = a^T x$ are **scalars**
  - a is a **vector**
  - Derivation:

$$f = x^T a = [x_1, x_2, \ldots, x_n] \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = a_1 x_1 + a_2 x_2 + \ldots + a_n x_n = \sum_{i=1}^{n} a_i x_i$$

$$\frac{\partial x^T a}{\partial x} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = a$$

Common Derivations

- $\nabla_x Ax = A^T$
- $\nabla_x x^T Ax = (A + A^T)x$
  - If W is **symetric**:
    - $\frac{\partial}{\partial s}(x - As)^T W(x - As) = -2A^T W(x - As)$
    - $\frac{\partial}{\partial x}(x - As)^T W(x - As) = 2W(x - As)$
- $\frac{\partial}{\partial A} \ln |A| = A^{-T}$
- $\frac{\partial}{\partial A} Tr[AB] = B^T$

The Chain Rule

- Let

$$f(x) = h(g(x))$$
$$x \in \mathbb{R}^n$$
$$f, g : \mathbb{R}^n \rightarrow \mathbb{R}$$
$$h : \mathbb{R} \rightarrow \mathbb{R}$$

- $\nabla f = h' \cdot \nabla g$

Exercise 1 - The Chain Rule

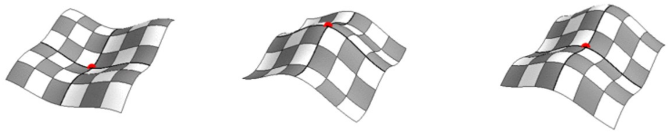
Find the gradient of $f(x) = \sqrt{x^T Q x}$ (Q is positive definite)

Solution 1

- $g(x) = x^T Q x \rightarrow \nabla g = (Q + Q^T)x = 2Qx$
- $h(z) = \sqrt{z} \rightarrow h'(z) = \frac{1}{2\sqrt{z}}$
- $\nabla f = \frac{1}{2\sqrt{x^T Q x}} 2Qx = \frac{Qx}{\sqrt{x^T Q x}}$

Multi-Dimensional Optimization

Optimality Conditions

- If f has *local* optimum at x_0 then $\nabla f(x_0) = 0$
- If the **Hessian** is:
  - **Positive Definite** (all eigenvalues *positive*) at $x_0 \rightarrow$ *local minimum*
  - **Negative Definite** (all eigenvalues *negative*) at $x_0 \rightarrow$ *local maximum*
  - Both **positive and negative** eigenvalues at $x_0 \rightarrow$ *saddle* point
  - 

Example - (Multivariate) Linear Least Squares

- **Problem Formulation**
  - $y \in \mathbb{R}^N$ - vector of values
  - $X \in \mathbb{R}^{N \times L}$ - data matrix with N examples and L *features*
  - $w \in \mathbb{R}^L$ - the *parameters* to be learnt, a **weight for each feature**
- **Goal**: find w that best fits the measurement y, that is, find a *weighted linear combination* of the feature vector to best fit the measurment y
- Mathematiacally, the problem is:

$$\min_w f(w; x, y) = \min_w \sum_{i=1}^{N} ||x_i w - y_i||^2$$

- In vector form:

$$\min_w f(w; x, y) = \min_w ||Xw - Y||^2$$

(Multivariate) LLS - Analytical Solution

- Mathematically:

$$\min_w f(w; x, y) = \min_w ||Xw - Y||^2 = \min_w (Xw - Y)^T (Xw - Y) = \min_w (w^T X^T X w - 2w^T X^T Y + Y^T Y)$$

- The derivative:

$$\nabla_w f(w; x, y) = (X^T X + X^T X)w - 2X^T Y = 0 \rightarrow w = (X^T X)^{-1} X^T Y$$
$$X^T X \in \mathbb{R}^{L \times L}$$

In [13]:
```python
# let's load the cancer dataset
dataset = pd.read_csv('./datasets/cancer_dataset.csv')
# print the number of rows in the data set
number_of_rows = len(dataset)
# reminder, the data looks like this
dataset.sample(10)
```

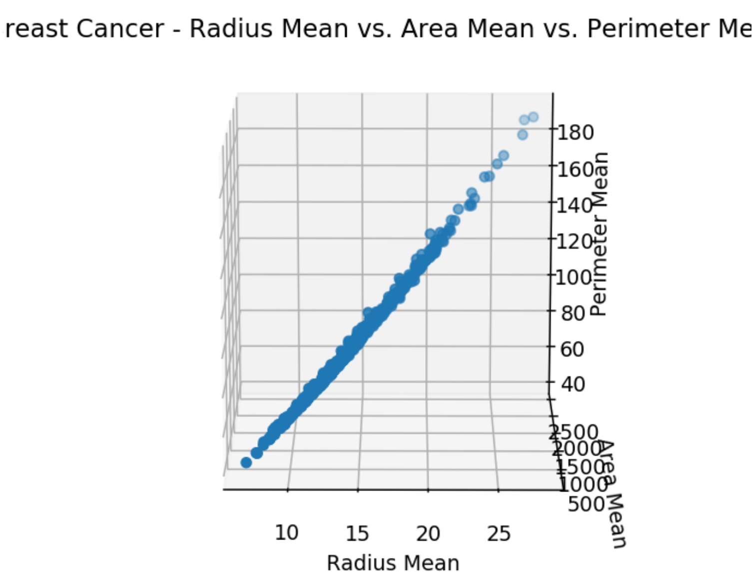
Out[13]:

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity
321	894618	M	20.16	19.66	131.10	1274.0	0.08020	0.08564	(
109	864018	B	11.34	21.26	72.48	396.5	0.08759	0.06575	(
448	911150	B	14.53	19.34	94.25	659.7	0.08388	0.07800	(
38	855133	M	14.99	25.20	95.54	698.8	0.09387	0.05131	(
384	902727	B	13.28	13.72	85.79	541.8	0.08363	0.08575	(
162	871201	M	19.59	18.15	130.70	1214.0	0.11200	0.16660	(
94	862028	M	15.06	19.83	100.30	705.6	0.10390	0.15530	(
24	852552	M	16.65	21.38	110.00	904.6	0.11210	0.14570	(
52	857374	B	11.94	18.24	75.71	437.6	0.08261	0.04751	(
562	925622	M	15.22	30.62	103.40	716.9	0.10480	0.20870	(

10 rows × 33 columns

In [14]:
```python
def plot_3d(x, y, z):
    %matplotlib notebook
    fig = plt.figure(figsize=(5, 5))
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(x, y, z)
    ax.set_xlabel('Radius Mean')
    ax.set_ylabel('Area Mean')
    ax.set_zlabel('Perimeter Mean')
    ax.set_title("Breast Cancer - Radius Mean vs. Area Mean vs. Perimeter Mean")
```

In [15]:
```python
# let's plot X = [radius, area], y = perimeter
xs = dataset[['radius_mean']].values
ys = dataset[['area_mean']].values
zs = dataset[['perimeter_mean']].values
plot_3d(xs, ys, zs)
```

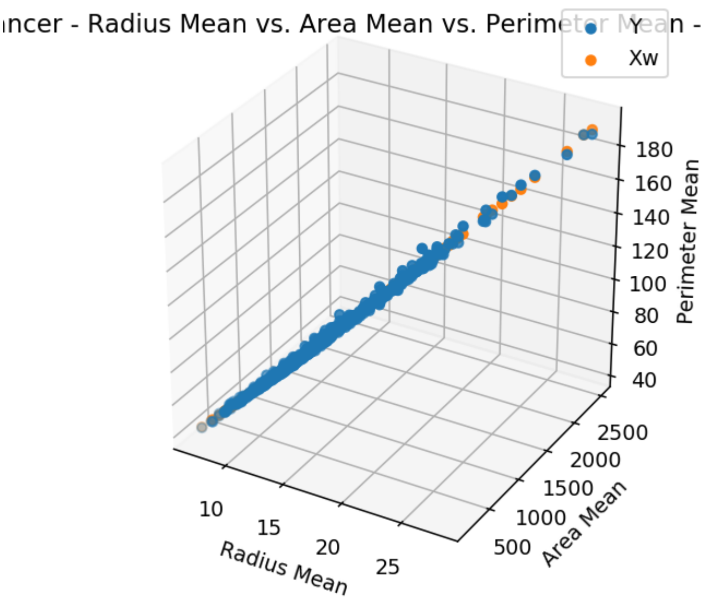


In [23]:
```
def plot_3d_lls(x, y, z, lls_sol, title=""):
    # plot
    %matplotlib notebook
    fig = plt.figure(figsize=(5, 5))
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(x, y, z, label='Y')
    ax.scatter(x, y, lls_sol, label='Xw')
    ax.legend()
    ax.set_xlabel('Radius Mean')
    ax.set_ylabel('Area Mean')
    ax.set_zlabel('Perimeter Mean')
    ax.set_title(title)
```

In [20]:
```
# multivariate lls - analytical solution
X = dataset[['radius_mean', 'area_mean']].values
Y = dataset[['perimeter_mean']].values
xs = dataset[['radius_mean']].values
ys = dataset[['area_mean']].values
zs = dataset[['perimeter_mean']].values
w = np.linalg.inv(X.T @ X) @ X.T @ Y
lls_sol = X @ w
print("w:")
print(w)
```

```
w:
[[6.19721311]
 [0.00676913]]
```

In [24]:
```
# plot
plot_3d_lls(xs, ys, zs, lls_sol, "Breast Cancer - Radius Mean vs. Area Mean vs. Perimeter Mean - LLS Analy
itical")
```



What If L is Very Large???

If $L = 1000$, we would need to invert a 1000×1000 matrix, which would take about 10^9 operations!

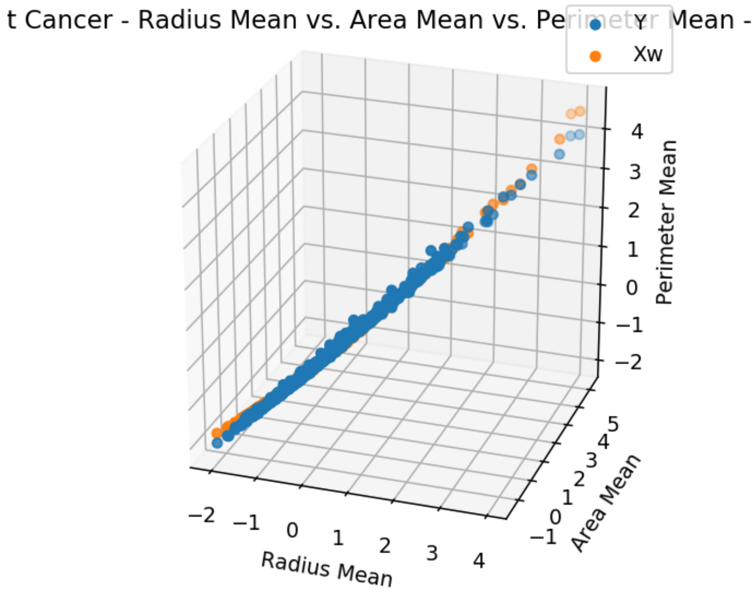
(Batch) Gradient Descent

- **Pseudocode**:
  - **Require**: Learning rate α_k
  - **Require**: Initial parameter vector w
  - **While** stopping criterion not met **do**
    - Compute gradient: $g \leftarrow \nabla f(x, w)$
    - Apply update: $w \leftarrow w - \alpha_k g$
    - $k \leftarrow k + 1$
  - **end while**

- For **Linear Least Squares**:
  - **Require**: Learning rate α_k
  - **Require**: Initial parameter vector w
  - **While** stopping criterion not met **do**
    - Compute gradient: $g \leftarrow 2X^T Xw - 2X^T y$
    - Apply update: $w \leftarrow w - \alpha_k g$
    - $k \leftarrow k + 1$
  - **end while**

In [ ]:
```python
# multivariate lls - gradient descent solution
X = dataset[['radius_mean', 'area_mean']].values
Y = dataset[['perimeter_mean']].values
# Scaling
X = (X - X.mean(axis=0, keepdims=True)) / X.std(axis=0, keepdims=True)
Y = (Y - Y.mean(axis=0, keepdims=True)) / Y.std(axis=0, keepdims=True)
num_iterations = 20
alpha_k = 0.0001
L = X.shape[1]
# initialize w
w = np.zeros((L, 1))
for i in range(num_iterations):
    print("iter:", i, " w = ")
    print(w)
    gradient = 2 * X.T @ X @ w - 2 * X.T @ Y
    w = w - alpha_k * gradient
lls_sol = X @ w
print("w:")
print(w)
```

In [34]:
```python
# plot
plot_3d_lls(X[:,0], X[:, 1], Y, lls_sol, "Breast Cancer - Radius Mean vs. Area Mean vs. Perimeter Mean - LLS GD")
```



Stochastic Gradient Descent (Mini-Batch Gradient Descent)

- **Pseudocode**:
  - **Require**: Learning rate α_k
  - **Require**: Initial parameter w
  - **While** stopping criterion not met **do**
    - Sample a minibatch of m examples from the training set ($m = 1$ for SGD)
    - Set $\tilde{X} = [x_1, \ldots, x_m]$ with corresponding targets $\tilde{Y} = [y_1, \ldots, y_m]$
    - Compute gradient: $g \leftarrow 2\tilde{X}^T\tilde{X} - 2\tilde{X}^T\tilde{Y}$
    - Apply update: $w \leftarrow w - \alpha_k g$
    - $k \leftarrow k + 1$
  - **end while**

In [36]:
```python
def batch_generator(x, y, batch_size, shuffle=True):
    """
    This function generates batches for a given dataset x.
    """
    N, L = x.shape
    num_batches = N // batch_size
    batch_x = []
    batch_y = []
    if shuffle:
        # shuffle
        rand_gen = np.random.RandomState(0)
        shuffled_indices = rand_gen.permutation(np.arange(N))
        x = x[shuffled_indices, :]
        y = y[shuffled_indices, :]
    for i in range(N):
        batch_x.append(x[i, :])
        batch_y.append(y[i, :])
        if len(batch_x) == batch_size:
            yield np.array(batch_x).reshape(batch_size, L), np.array(batch_y).reshape(batch_size, 1)
            batch_x = []
            batch_y = []
    if batch_x:
        yield np.array(batch_x).reshape(-1, L), np.array(batch_y).reshape(-1, 1)
```

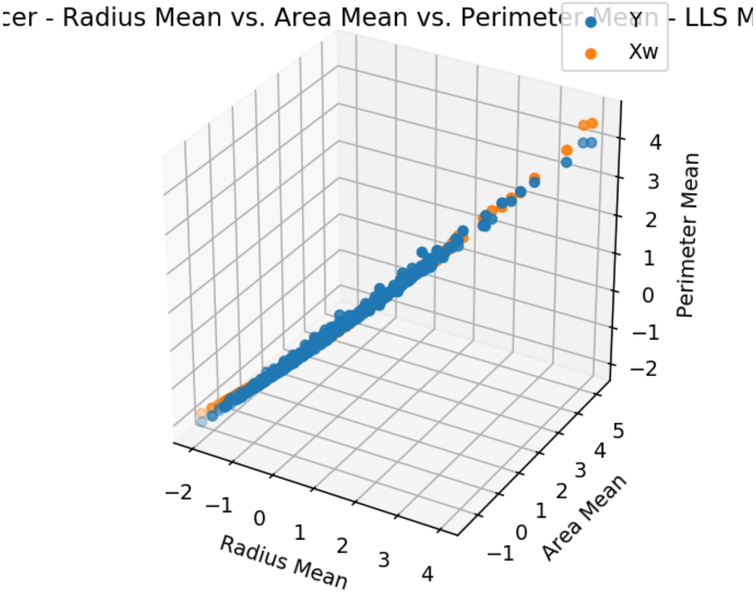
In [37]:
```
# multivaraite mini-batch gradient descent
X = dataset[['radius_mean', 'area_mean']].values
Y = dataset[['perimeter_mean']].values
# Scaling
X = (X - X.mean(axis=0, keepdims=True)) / X.std(axis=0, keepdims=True)
Y = (Y - Y.mean(axis=0, keepdims=True)) / Y.std(axis=0, keepdims=True)
N = X.shape[0]
batch_size = 10
num_batches = N // batch_size
print("total batches:", num_batches)
```

```
total batches: 56
```

In [ ]:
```
num_iterations = 10
alpha_k = 0.001
batch_gen = batch_generator(X, Y, batch_size, shuffle=True)
# initialize w
w = np.zeros((L, 1))
for i in range(num_iterations):
    for batch_i, batch in enumerate(batch_gen):
        batch_x, batch_y = batch
        if batch_i % 50 == 0:
            print("iter:", i, "batch:", batch_i, " w = ")
            print(w)
        gradient = 2 * batch_x.T @ batch_x @ w - 2 * batch_x.T @ batch_y
        w = w - alpha_k * gradient
    batch_gen = batch_generator(X, Y, batch_size, shuffle=True)

lls_sol = X @ w
```

In [39]:
```
# plot
plot_3d_lls(X[:,0], X[:, 1], Y, lls_sol, "Breast Cancer - Radius Mean vs. Area Mean vs. Perimeter Mean - L
LS Mini-Batch GD")
print("w:")
print(w)
```




```
w:
[[0.55894282]
 [0.42792729]]
```

Constrained Optimization

Largrange Multipliers

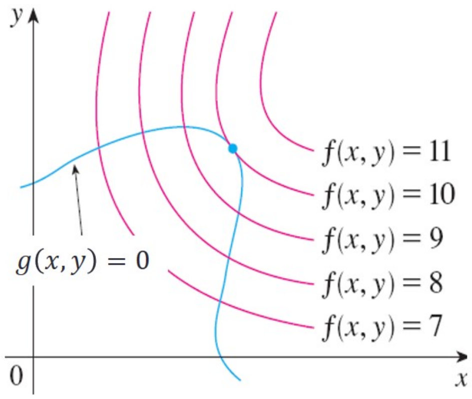
- A method for optimization with **equality constraints**
- The general case:

$$\min f(x,y)$$
$$s.t. \ (subject \ to): g(x,y) = 0$$

- The *Lagrange* function (*Lagrangian*) is defined by:

$$\mathcal{L}(x,y,\lambda) = f(x,y) - \lambda \cdot g(x,y)$$

- Geometric Intuition: let's look at the following figure -



- The blue line shows the constraint $g(x,y) = 0$
- The red lines are contours of $f(x,y) = c$
- The point where the blue line tangentially touches a red contour is the maximum of $f(x,y) = c$ that satisfy the constraint $g(x,y) = 0$

- To maximize $f(x,y)$ subject to $g(x,y) = 0$ is to find the largest value $c \in \{7, 8, 9, 10, 11\}$ such that the level curve (contour) $f(x,y) = c$ intersects with $g(x,y) = 0$
- It happens when the curves just touch each other
  - When they have a common tangent line
- Otherwise, the value of c should be increased

- Since the gradient of a function is **perperndicular** to the contour lines:
  - The *contour lines* of f and g are **parallel** iff the *gradients* of f and g are **parallel**
  - Thus, we want points (x,y) where $g(x,y) = 0$ and

$$\nabla_{x,y} f(x,y) = \lambda \nabla_{x,y} g(x,y)$$

    - λ - "The Lagrange Multiplier" is required to adjust the **magnitudes** of the (parallel) gradient vectors.

Multiple Constraints

- Extenstion of the above for problems with **multiple constraints** using a similar argument
- The general case: minimize $f(x)$ s.t. $g_i(x) = 0$, $i = 1, 2, \ldots, m$
- The **Lagrangian** is a weighted sum of objective and constraint functions:

$$\mathcal{L}(x, \lambda_1, \ldots, \lambda_m) = f(x) - \sum_{i=1}^{m} \lambda_i g_i(x)$$

  - λ_i is the Lagrange multipler associated with $g_i(x) = 0$

- The **solution** is obtained by solving the (unconstrained) optimization problem:

$$\nabla_{x,\lambda_1,\ldots,\lambda_m} \mathcal{L}(x, \lambda_1, \ldots, \lambda_m) = 0 \iff \begin{cases} \nabla_x \left[f(x) - \sum_{i=1}^{m} \lambda_i g_i(x) = 0 \right] \\ g_1(x) = \ldots = g_m(x) = 0 \end{cases}$$

  - Amounts to solving $d + m$ equations in $d + m$ unknowns
    - $d = |x|$ is the dimension of x

Exercise 2 - Max Entropy Distribution

Maximize $H(P) = -\sum_{i=1}^{d} p_i \log p_i$ subject to $\sum_{i=1}^{d} p_i = 1$

Solution 2

- The Lagrangian is:

$$L(P, \lambda) = -\sum_{i=1}^{d} p_i \log p_i - \lambda\left(\sum_{i=1}^{d} p_i - 1\right)$$

- Find stationary point for L:
  - $\forall i, \frac{\partial L(P,\lambda)}{\partial p_i} = -\log p_i - 1 - \lambda = 0 \rightarrow p_i = e^{-\lambda-1}$
  - $\frac{\partial L(P,\lambda)}{\partial \lambda} = -\sum_{i=1}^{d} p_i + 1 = 0 \rightarrow \sum_{i=1}^{d} e^{-\lambda-1} = 1 \rightarrow e^{-\lambda-1} = \frac{1}{d} = p_i$
  - The Max Entropy distribution is the **uniform distribution**

Recommended Videos

Warning!

- These videos do not replace the lectures and tutorials.
- Please use these to get a better understanding of the material, and not as an alternative to the written material.

Video By Subject

- Gradient Descent - [Gradient Descent, Step-by-Step (https://www.youtube.com/watch?v=sDv4f4s2SB8)](https://www.youtube.com/watch?v=sDv4f4s2SB8)
  - [Mathematics of Gradient Descent - Intelligence and Learning (https://www.youtube.com/watch?v=jc2IthslyzM)](https://www.youtube.com/watch?v=jc2IthslyzM)
- Stochastic Gradient Descent - [Stochastic Gradient Descent, Clearly Explained (https://www.youtube.com/watch?v=vMh0zPT0tLI)](https://www.youtube.com/watch?v=vMh0zPT0tLI)
- Constrained Optimization - [Constrained Optimization with LaGrange Multipliers (https://www.youtube.com/watch?v=nUfYR5FBGZc)](https://www.youtube.com/watch?v=nUfYR5FBGZc)
- Lagrange Multipliers - [Lagrange Multipliers I Geometric Meaning & Full Example (https://www.youtube.com/watch?v=8mjcnxGMwFo)](https://www.youtube.com/watch?v=8mjcnxGMwFo)

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