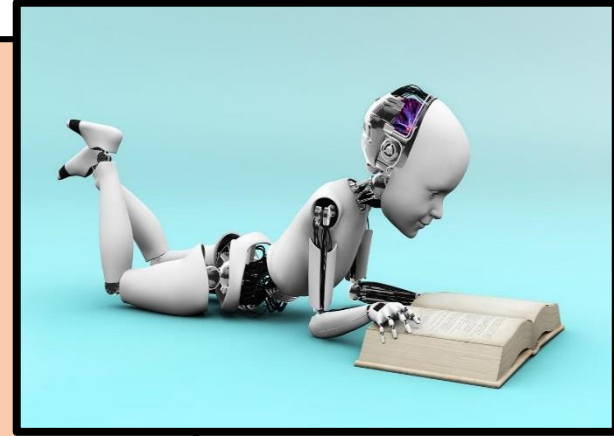


Machine learning from data

Class1: Linear Regression



Zohar Yakhini
IDC



Example: House Pricing



- We want to know the price of a house as a function of its size (in sqft).
- We want to learn a function from the size of the house x to the price $y = f(x)$ so we would be able to answer the above question
- Training set: 10 house instances with feature values and labels

Square Feet (x)	House Price in \$1000s (y)
1400	245
1600	312
1700	279
1875	308
1100	199
1550	219
2350	405
2450	324
1425	319
1700	255

Statistics:

Dependent variable (y) = house price

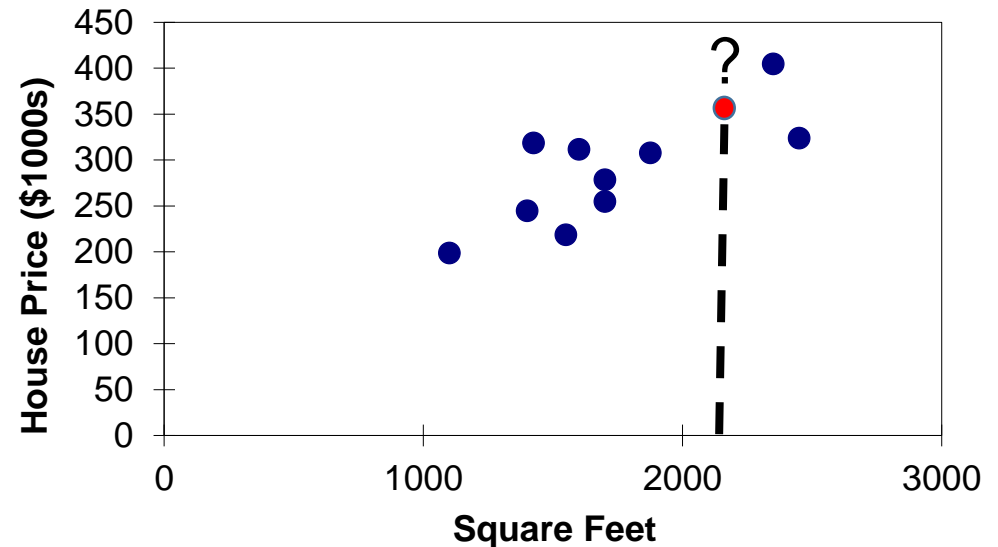
Explaining variable (x) = square footage

Graphical Representation

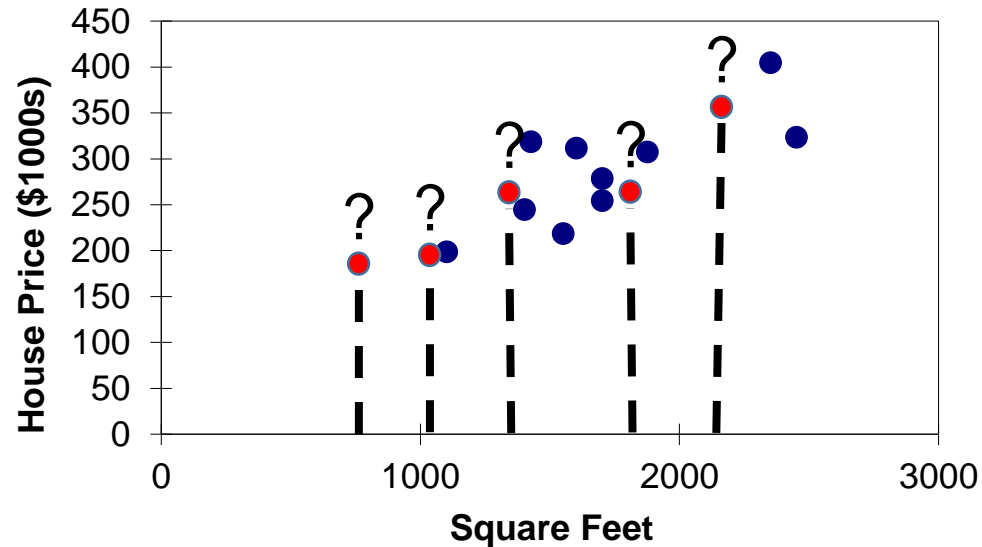
Scatter plot of
House Price (y) vs
House Size (x)

Prediction:

Given house of size x ,
what would be its
price $y = f(x)$?

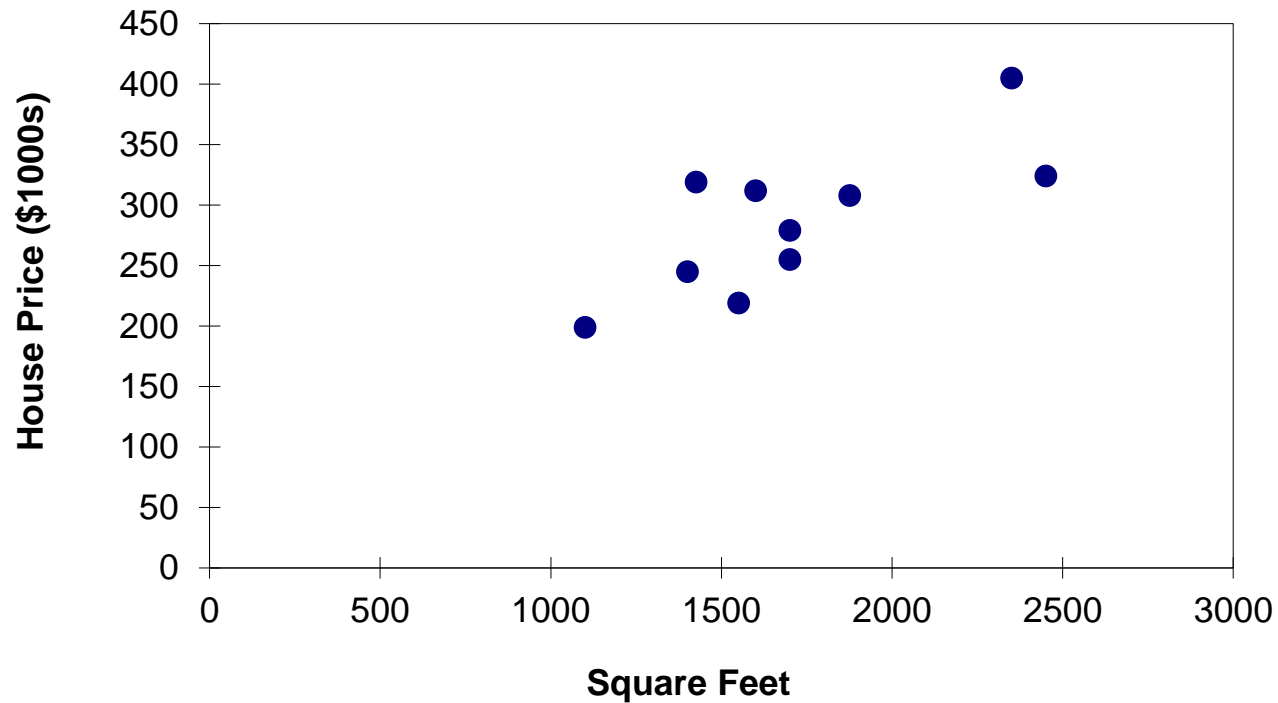


Memorization?

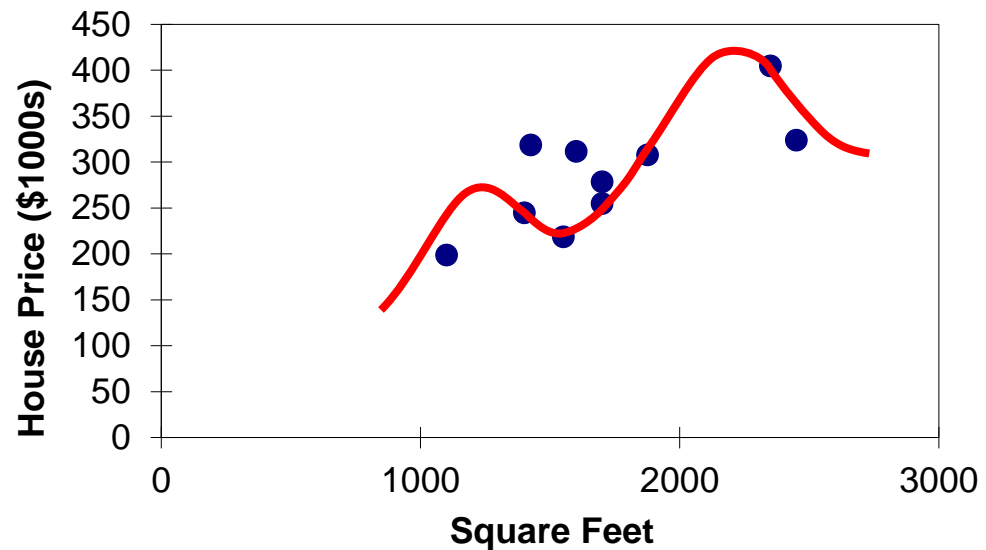


- Store all sizes?
- Our data doesn't cover all sizes ... What shall we do w a house of size 1750 sqft?

OK ... a function?

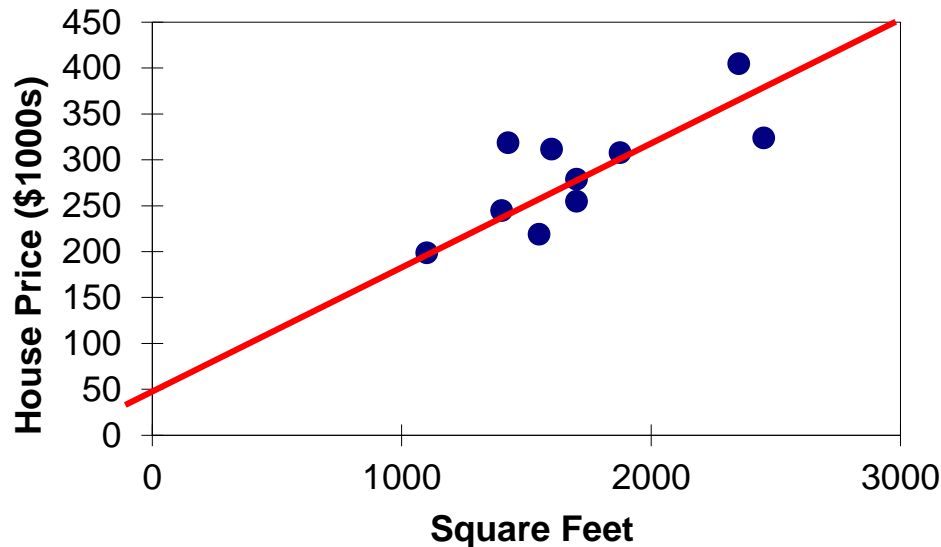


Generalization: Learn a Function



But which function $y=f(x)$?

Simplest: Linear Model



- We assume/hypothesize that the relationship between the observed and the independent/explained variable is linear and thereby conduct our search
- This is our **Hypotheses Space** – all linear functions

Linear Function Hypothesis

- How do we represent a hypothesis h in this space?

$$y = \theta_0 + \theta_1 x$$

- What if we have many features and not just house size?
- Such as:
 - Number of rooms
 - Distance to shopping center
 - Neighborhood crime rate
 - Distance to IDC
 - More...

Multiple Features; Higher Dimension

- Let $\mathbf{x}^{(i)} = (x_1^{(i)}, x_2^{(i)}, \dots, x_n^{(i)})$
be the vector of feature values for each instance i
- For simplicity we add another “constant” feature for every i

$$x_0^{(i)} = 1$$

- For n features our linear hypothesis will be represented by the parameters

$$\boldsymbol{\theta} = (\theta_0, \theta_1, \theta_2, \dots, \theta_n)$$

with which we construct:

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

- We say that $\boldsymbol{\theta} = (\theta_0, \theta_1, \theta_2, \dots, \theta_n)$

is the vector of parameters that defines our function
(or our **model/execution-algorithm/hypothesis**)

The Hypothesis (or model) is the execution algorithm

- How does a specific set of values,

$$\theta = (\theta_0, \theta_1, \theta_2, \dots, \theta_n)$$

which defines a specific hypothesis (model) help us?

- How can we use it?
- Given a new house instance $\mathbf{x}' = (x'_0, x'_1, \dots, x'_n)$ we can estimate its price by an inner product with the vector θ :

$$\text{value of house} = y = \theta_0 + \theta_1 x'_1 + \theta_2 x'_2 + \dots + \theta_n x'_n$$

Finding the Best Hypothesis/Model

- There are many possible parameter vectors

$$\theta = (\theta_0, \theta_1, \theta_2, \dots, \theta_n)$$

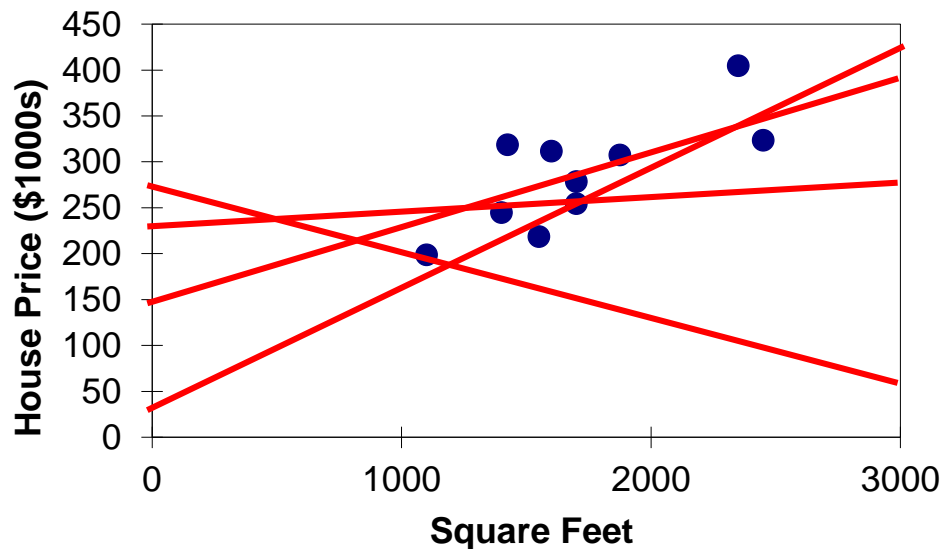
and each one defines a different hypothesis in our hypotheses space

- How do we find the best one?
- What can we use to help us find it?
- The training set: m instances where, for each, we know the feature values $\mathbf{x}^{(i)} = (x_0^{(i)}, x_1^{(i)}, \dots, x_n^{(i)})$ as well as the label value $y^{(i)}$

The Hypotheses Space

- For the simple case of a single feature we get different possible straight lines when we change θ_0 and θ_1 in the hypothesis (model)

$$y = \theta_0 + \theta_1 x$$

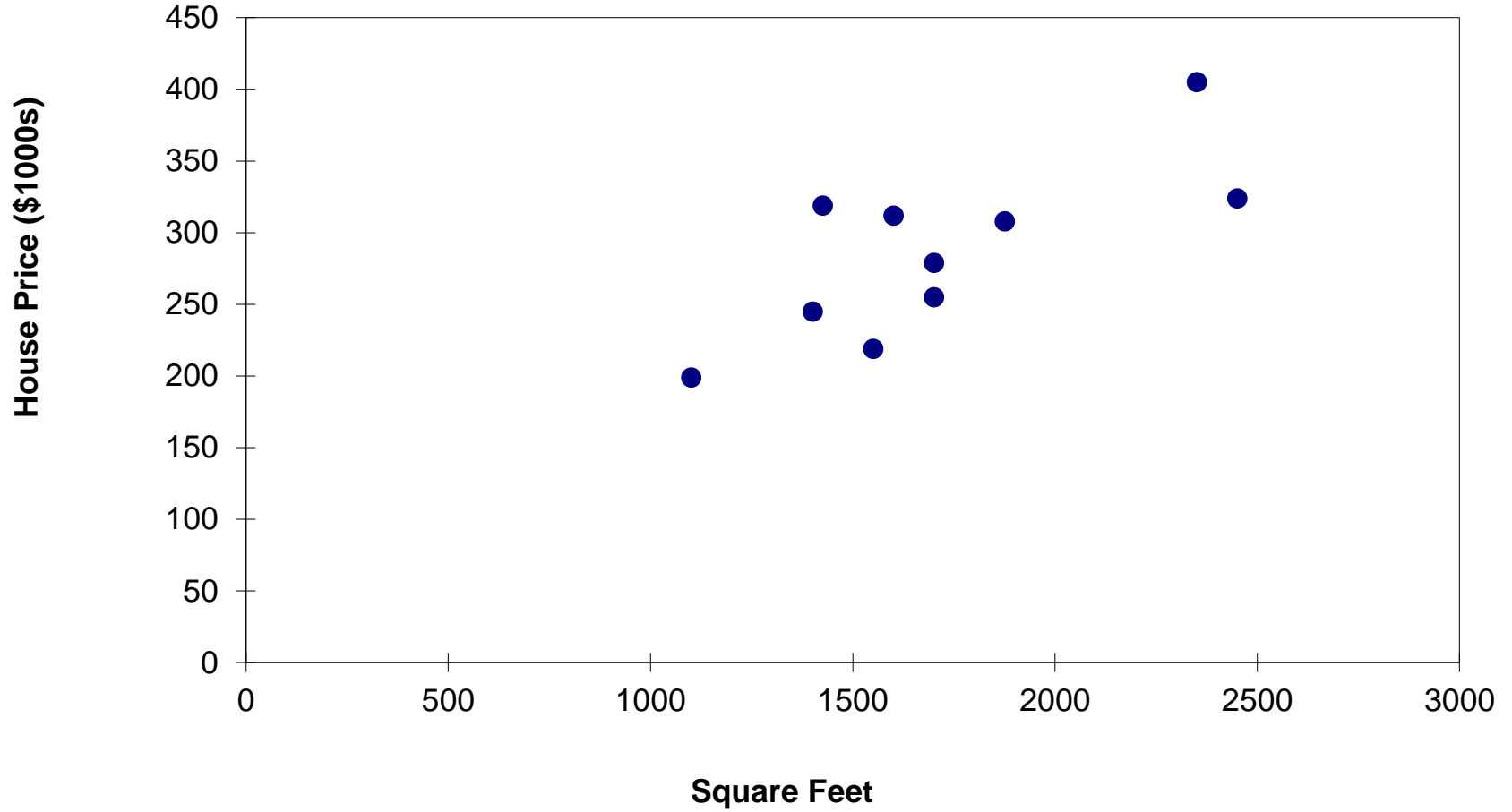


“Training” or “Learning”. ERM

- We require that on our training data the values of our prediction function (f) would be similar to the known value of the house.
- So, we want to find θ such that for all instances i in the training set we will have:

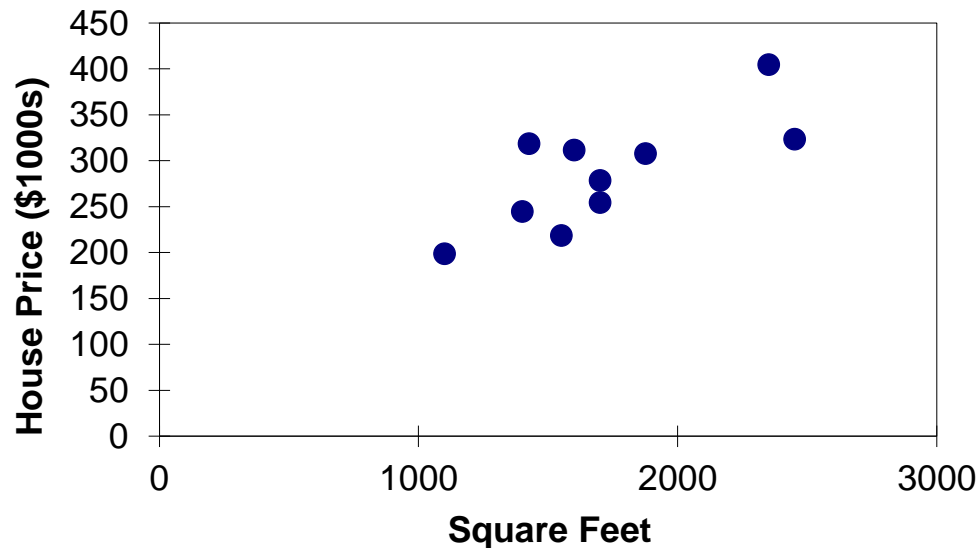
$$y^{(i)} = \theta_0 x_0^{(i)} + \theta_1 x_1^{(i)} + \theta_2 x_2^{(i)} + \dots + \theta_n x_n^{(i)} = \theta \cdot \mathbf{x}^{(i)}$$

- However, this may not always be possible – (why?)



Consistent Learners

- A learning algorithm that can achieve 0 error on the training set is called a “consistent learner”
- This can not be done here.



Cost Function of a Model θ

Prediction

*Actual
value*

- As consistent learning may be impossible.
- Still, we can try to reduce the error.
Per instance the error is:

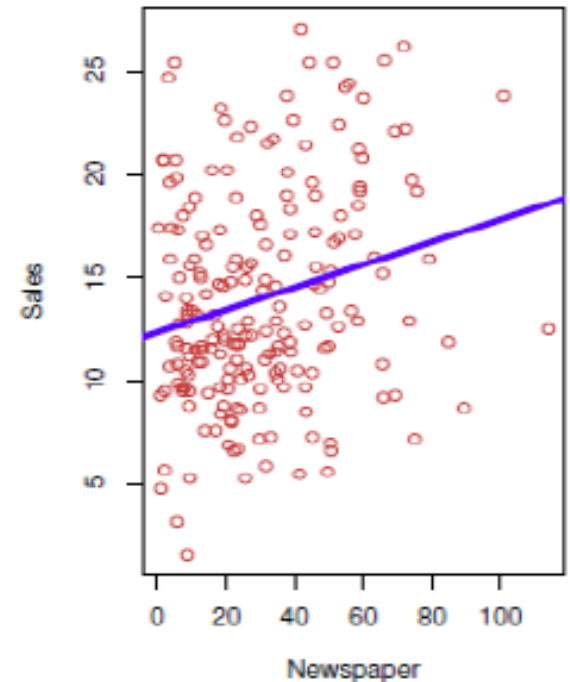
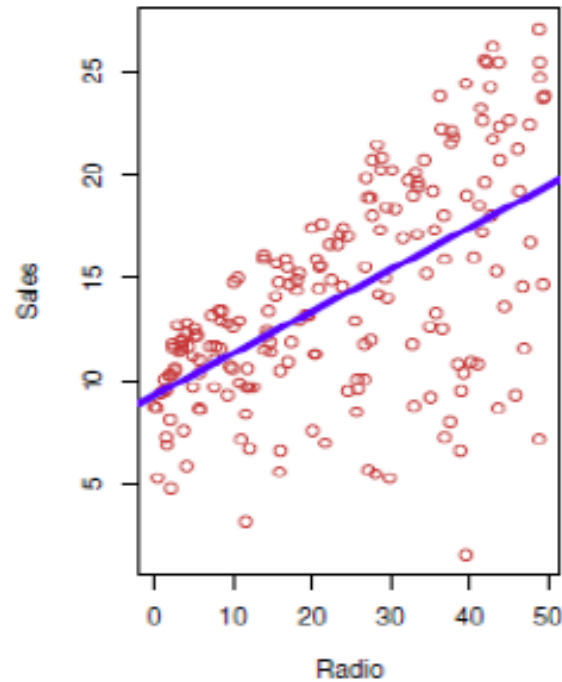
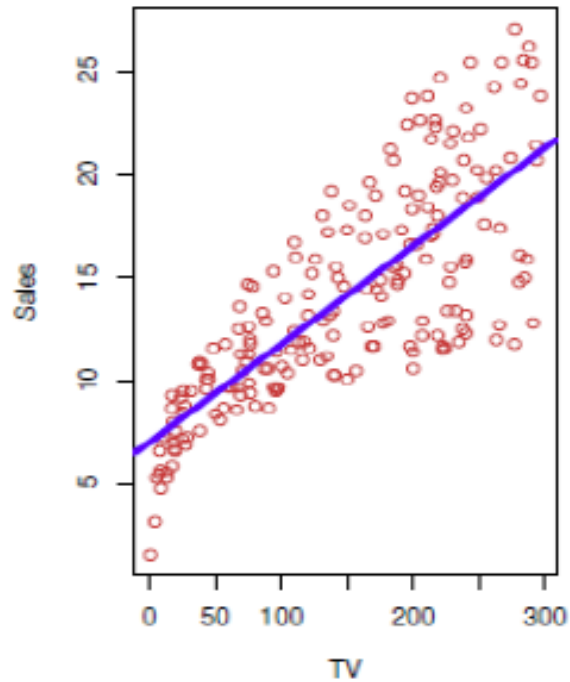
$$(\theta_0 x_0^{(i)} + \theta_1 x_1^{(i)} + \theta_2 x_2^{(i)} + \dots + \theta_n x_n^{(i)} - y^{(i)}) = \boxed{\theta \cdot \mathbf{x}^{(i)}} - \boxed{y^{(i)}}$$

- And we now average on ALL m training instances to get our **cost function**:

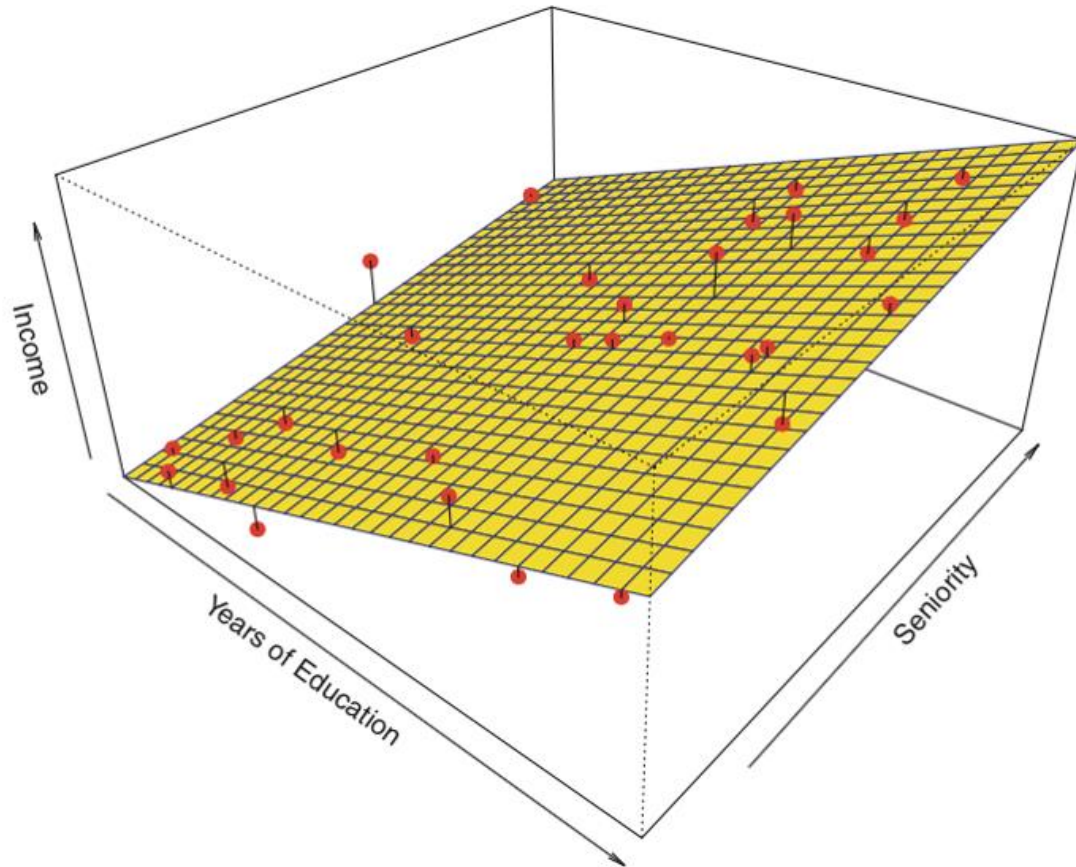
$$J(\theta) = \frac{1}{2} \frac{1}{m} \sum_{i=1}^m \left(\theta \cdot \mathbf{x}^{(i)} - y^{(i)} \right)^2$$

- Square errors are used so that errors in different directions don't cancel out ...
Its also a smoother function compared to $|x|$

Example: advertising and sales



In higher dimensions



Minimizing the Cost Function

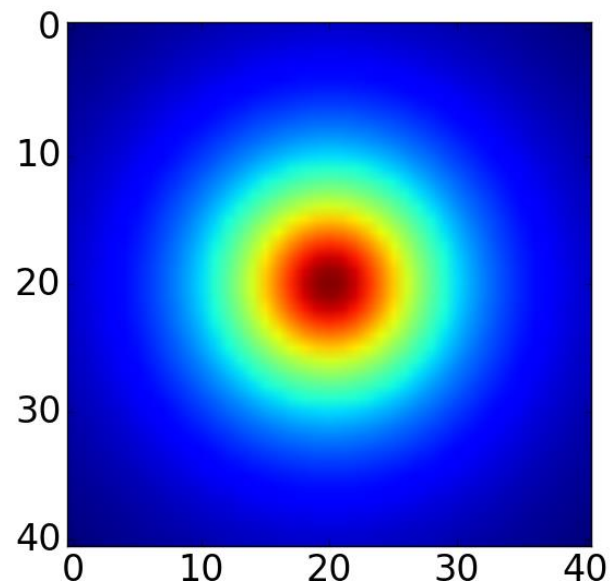
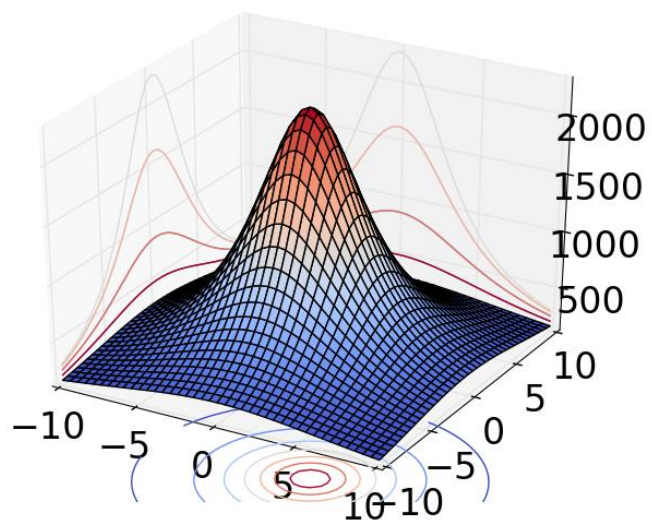
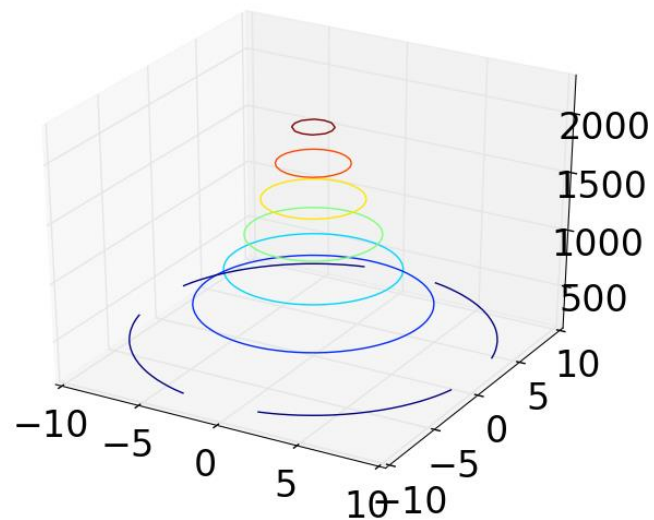
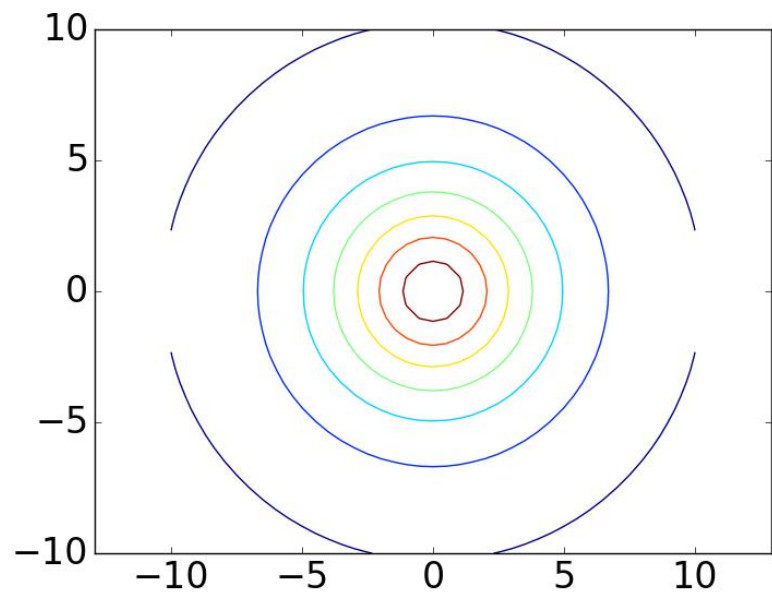
- In the ERM approach, our best hypothesis θ^* would be the one that minimizes the cost function. Formally:

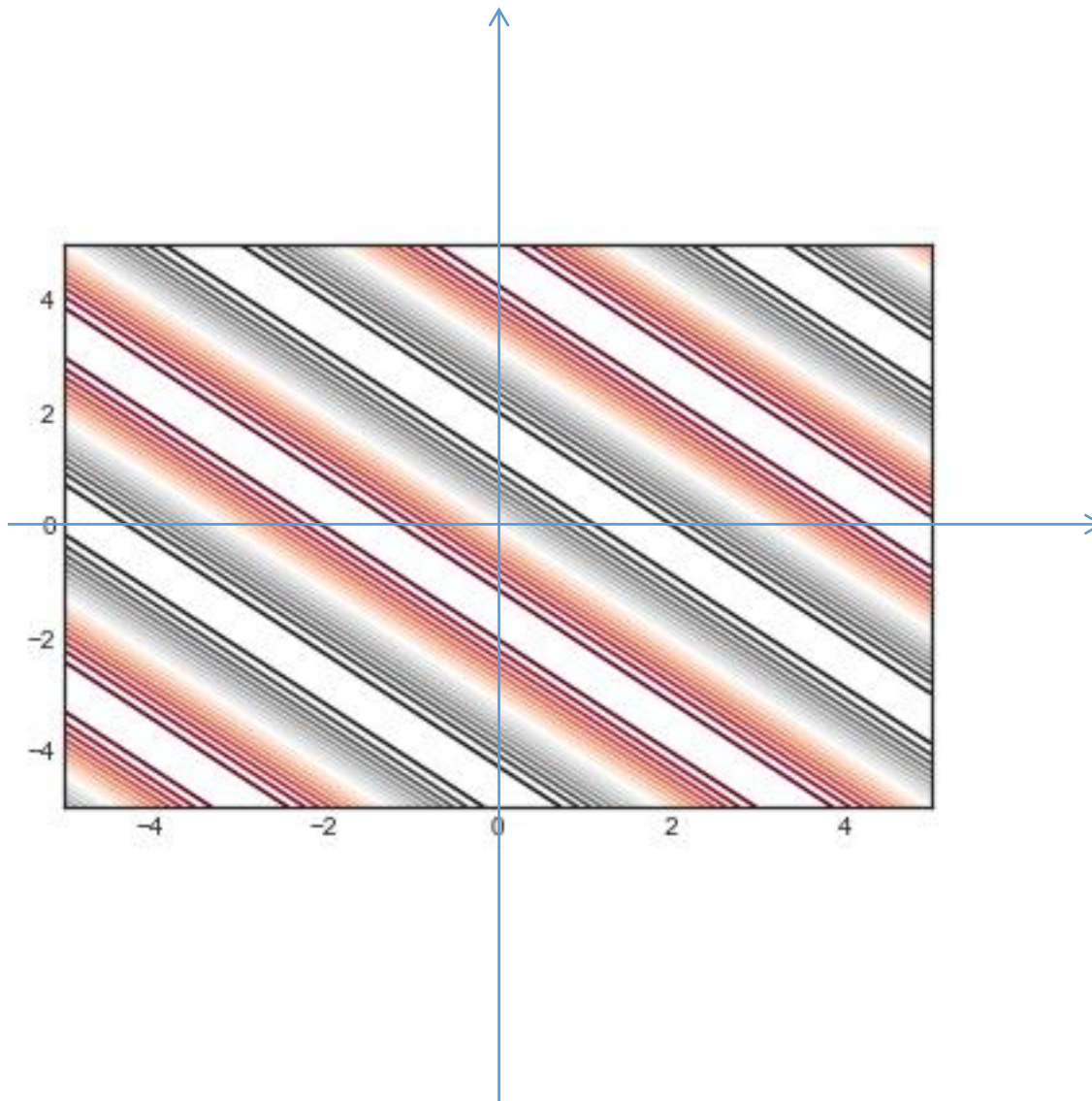
$$\theta^* = \arg \min_{\theta} [J(\theta)] = \arg \min_{\theta} \left[\frac{1}{2m} \sum_{i=1}^m (\theta \cdot \mathbf{x}^{(i)} - y^{(i)})^2 \right]$$

- How can we find it?

The Cost Function

- In our simple case (house prices) we have 2 parameters: θ_0, θ_1
- For each value of these two parameters we can calculate the cost $J(\theta_0, \theta_1)$ over the entire training data (the training error).
- This is a function from \mathbb{R}^2 to \mathbb{R} .





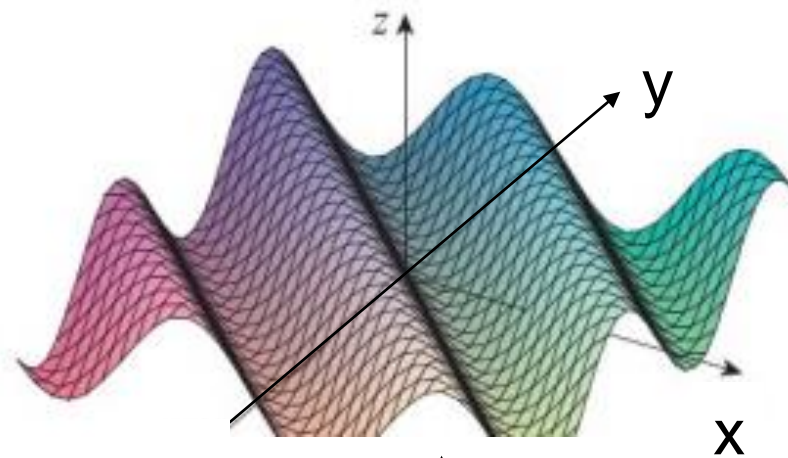
Code to generate the contour plot

```
def f(x, y):  
    return np.sin(x+y)
```

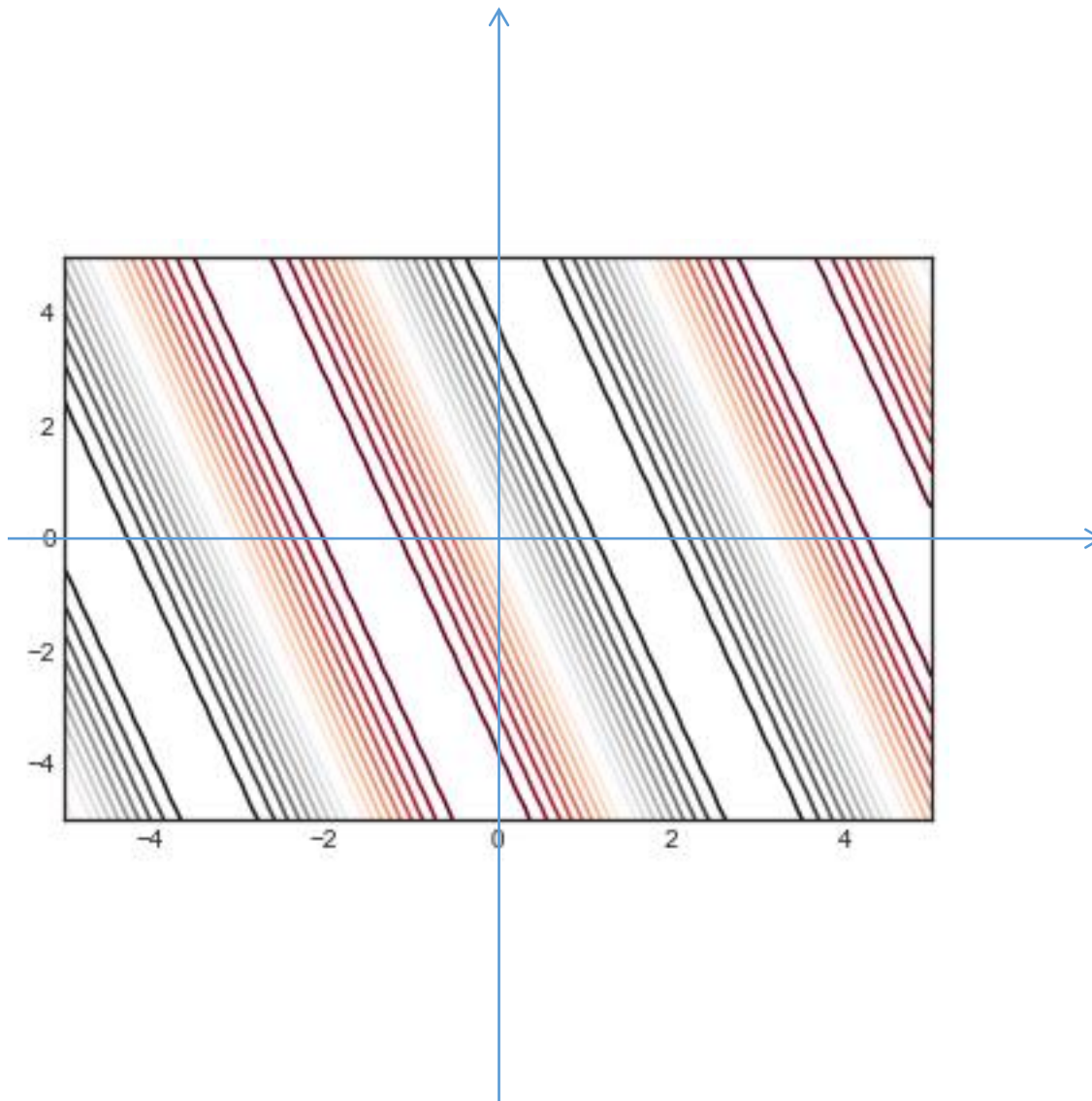
```
x = np.linspace(-5, 5, 50)  
y = np.linspace(-5, 5, 50)
```

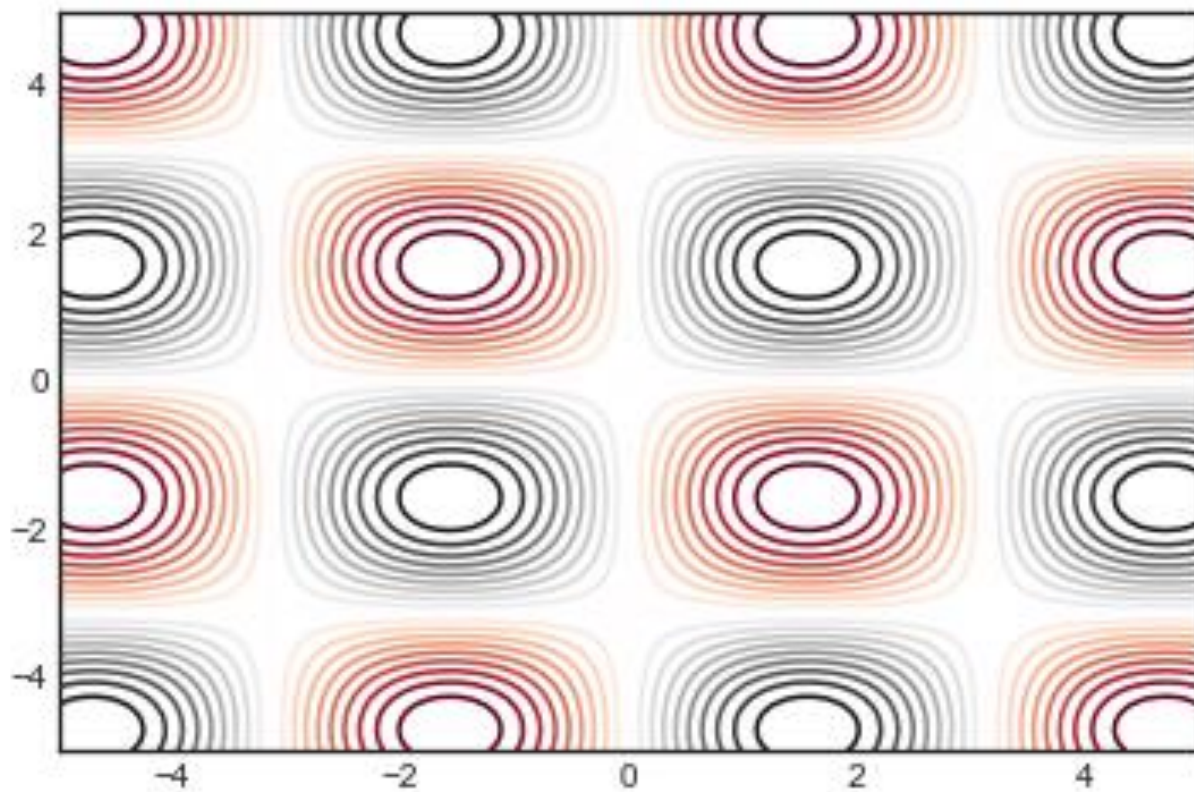
```
mx, my = np.meshgrid(x, y)  
z = f(mx, my)
```

```
plt.contour(mx, my, z, 20, cmap='RdGy');
```



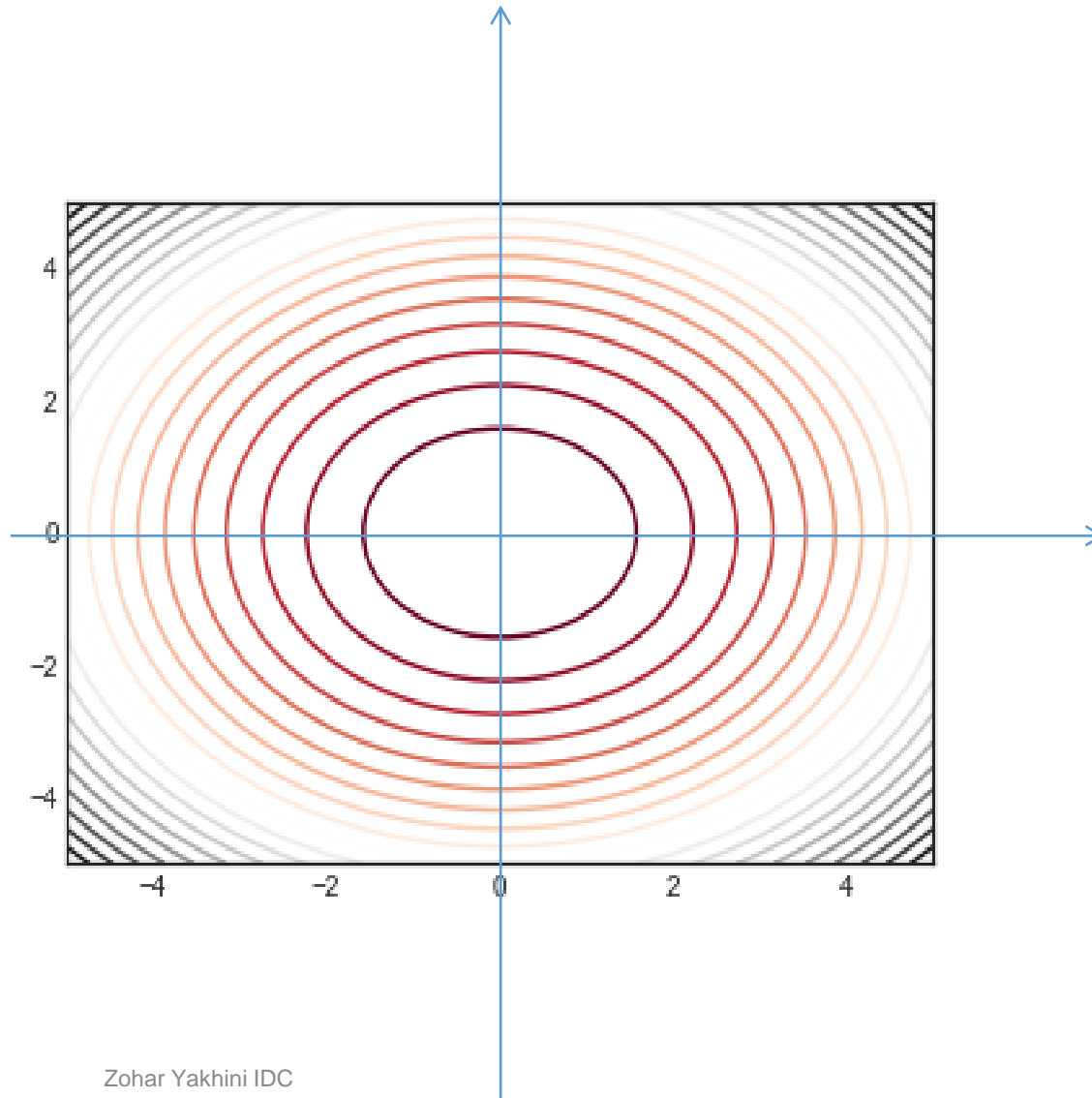
↑
3D plot.
Not a contour plot

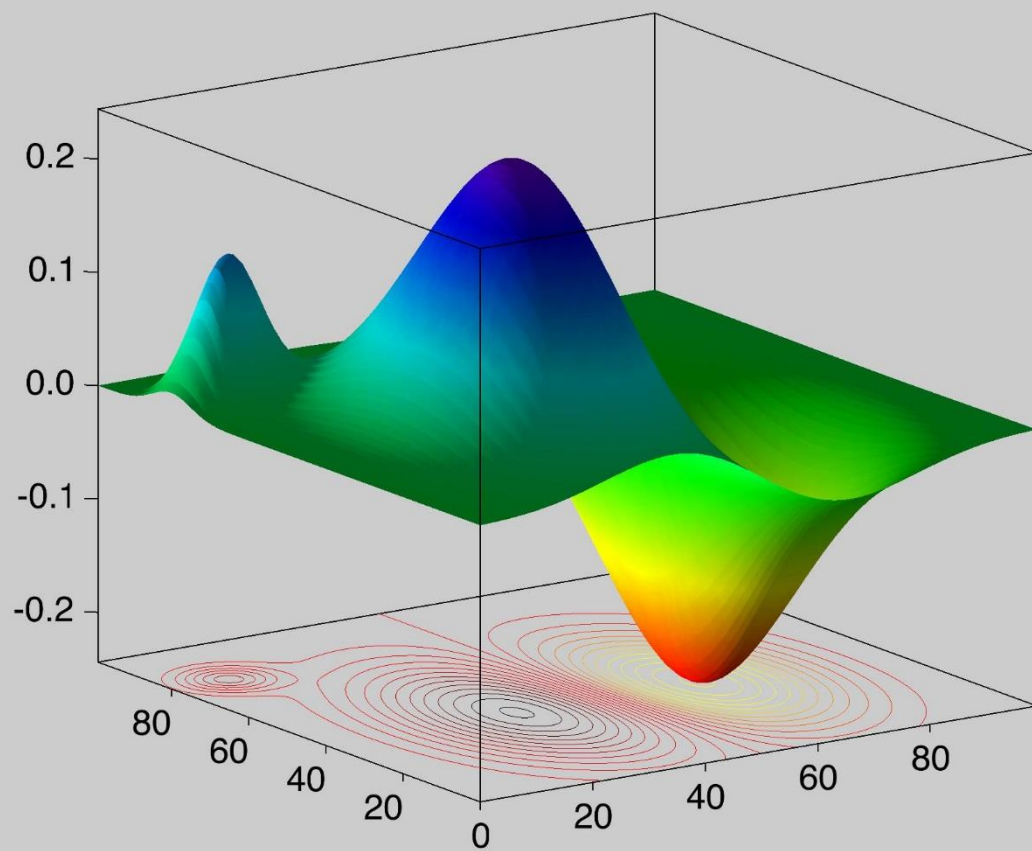




Recall:

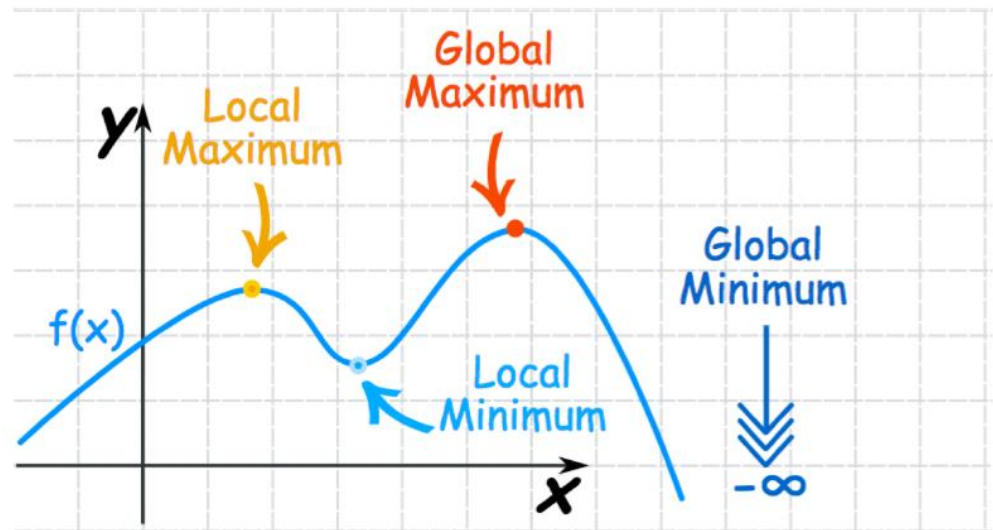
We want to find the argmin of the cost function $J(\theta)$





How to Find the Minimum of a 1D function?

- In high school:
derivative at the point where an extremum is attained
should be 0
- We can also follow the “downward” direction.
- How is this done?
 1. Find the derivative
 2. Move against its sign



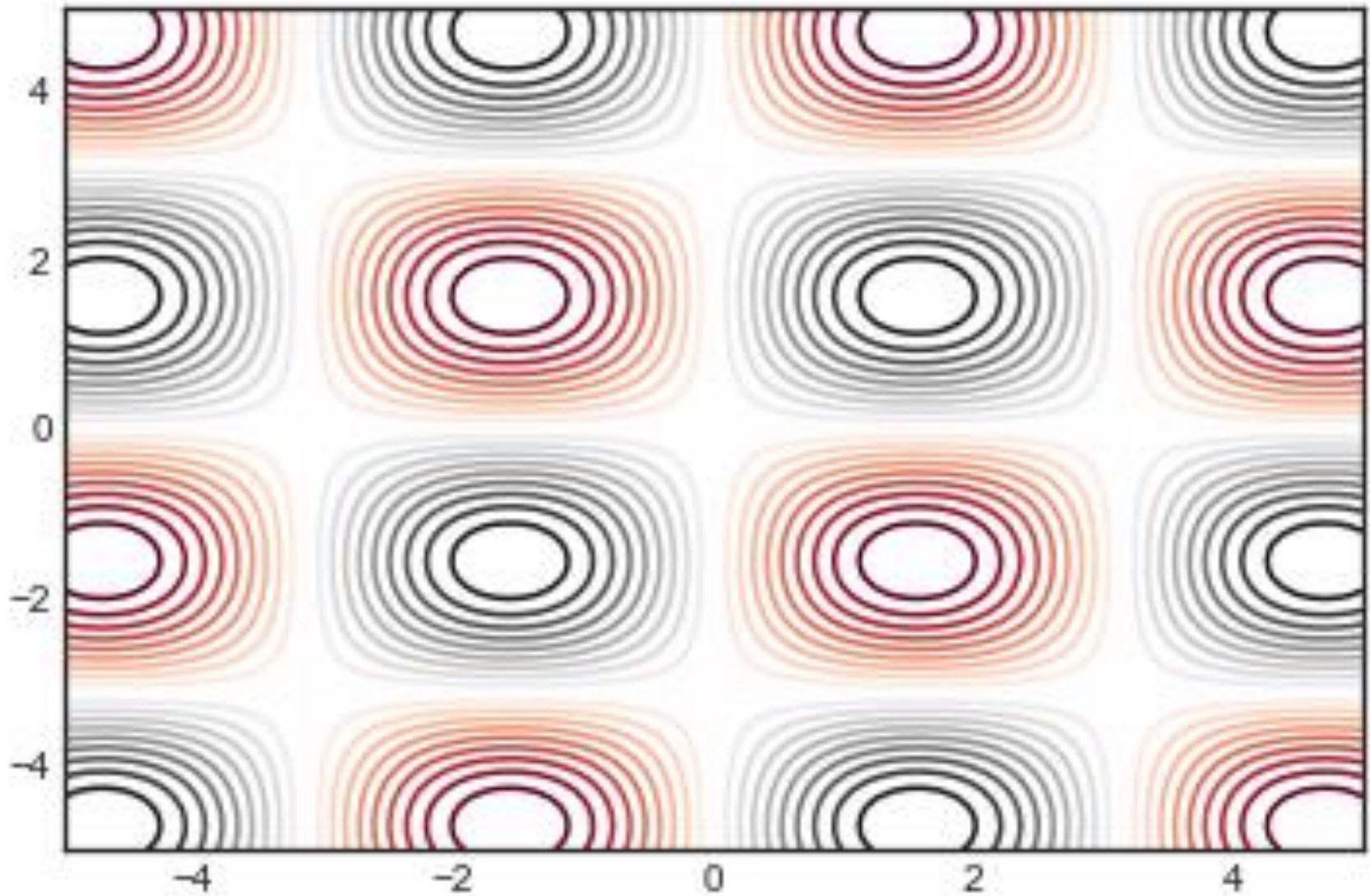
Directional Derivatives

Consider a differentiable 2D function $f(x_1, x_2)$. The derivative in a general direction $u = (u_1, u_2)$ (unit 2D vector) is called the directional derivative $D_u f$ and is defined as:

$$D_u f(x_1, x_2) = \lim_{s \rightarrow 0} \frac{f(x_1 + su_1, x_2 + su_2) - f(x_1, x_2)}{s} = \left(\frac{df}{ds} \right)_u$$

For a differentiable 2D function $f(x_1, x_2)$ the principal partial derivatives, those in direction $u = x_i$ are denoted

$$\frac{\partial f}{\partial x_1}(x_1, x_2) \text{ and } \frac{\partial f}{\partial x_2}(x_1, x_2)$$



Partial Derivatives

- Again, for a differentiable 2D function $f(x, y)$, the (principal) partial derivatives in the directions x and y are denoted

$$\frac{\partial f}{\partial x}(x, y), \frac{\partial f}{\partial y}(x, y)$$

- They can be computed by keeping one variable constant and differentiating by the other.
For example ...

$$\begin{aligned} f(x, y) &= 2x + 13y \\ f(x, y) &= y \exp(x) \\ f(x, y) &= 2x + 3xy + 5y^2 \end{aligned}$$

$$f(x, y) = y e^x$$

$$\frac{\partial f}{\partial x}(x, y) = y e^x$$

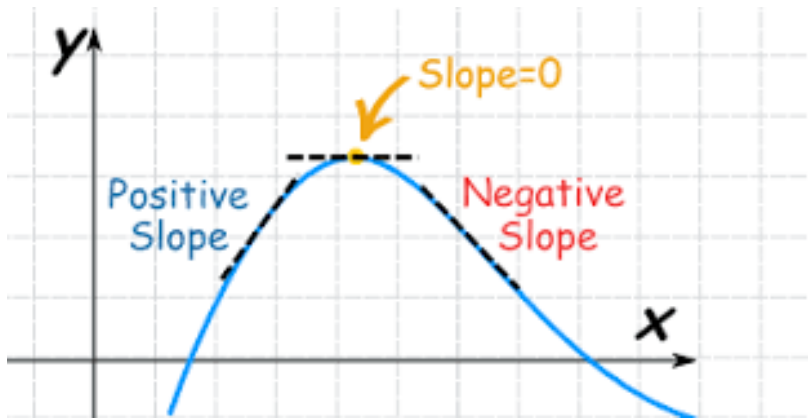
$$\frac{\partial f}{\partial y}(x, y) = e^x$$

$$f(x, y) = y^4 e^x$$

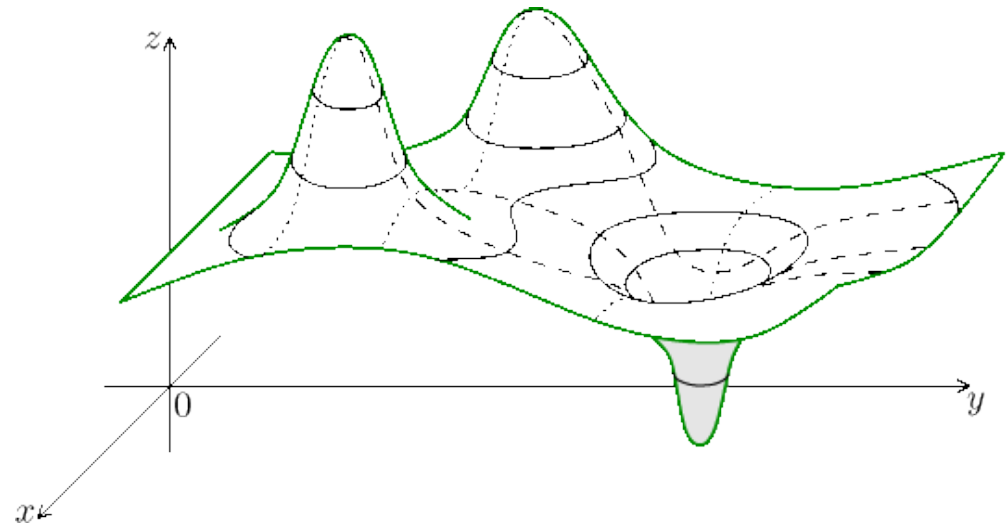
$$\frac{\partial f}{\partial x}(x, y) = y^4 e^x$$

$$\frac{\partial f}{\partial y}(x, y) = 4y^3 e^x$$

Extrema and zero derivatives



1D



2D

The Gradient of a function

Define the
GRADIENT of f :

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right)$$

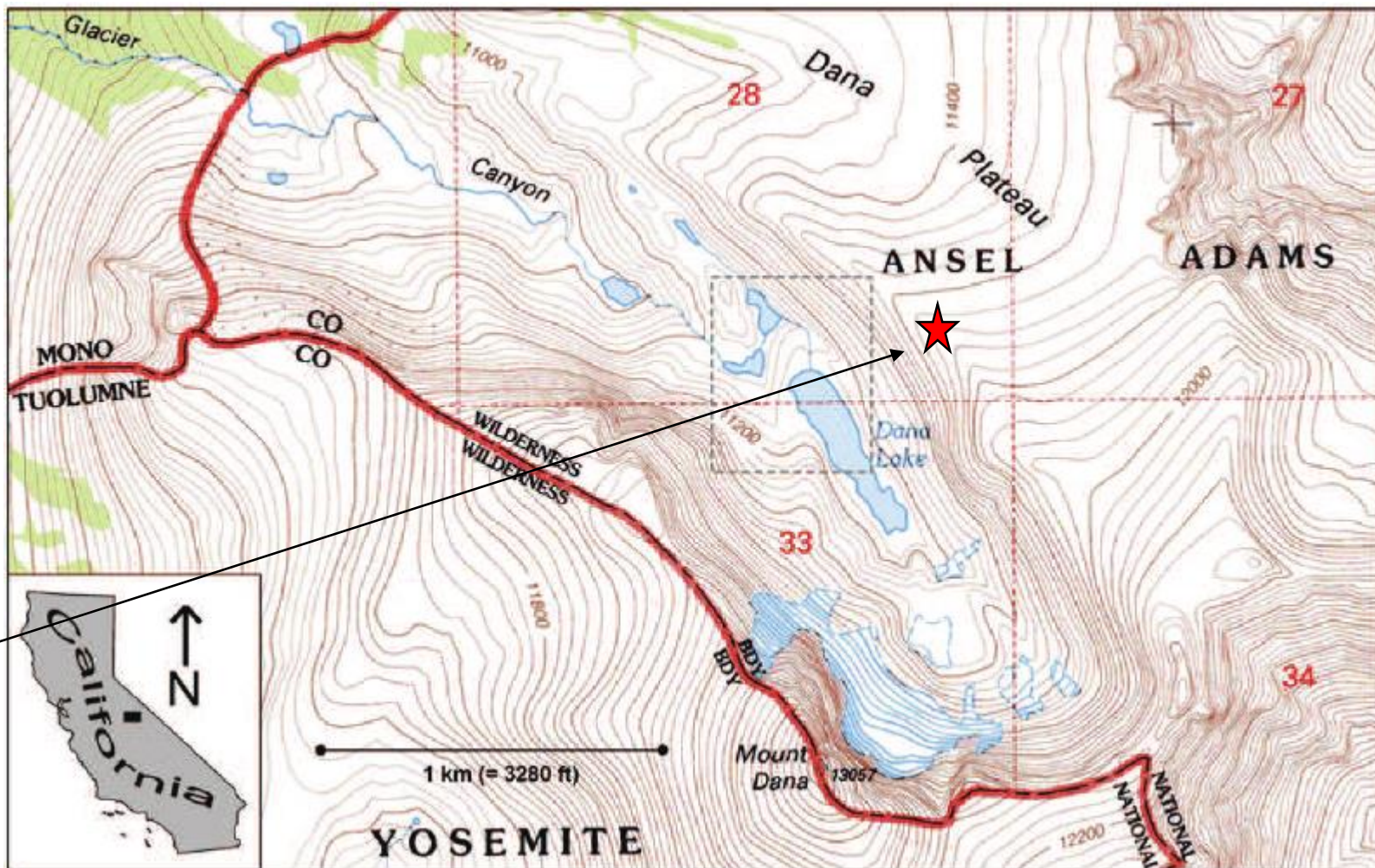
Thm:

For any direction $u = (u_1, u_2)$ and any point $\vec{x} = (x_1, x_2)$ we have:

$$D_u f(\vec{x}) = \langle \nabla f(\vec{x}), u \rangle$$

Most Rapid Increase at a point \vec{x} ?

The pt \vec{x}



Most Rapid Increase at a point \vec{x}

- The directional derivative in the direction of the vector $\mathbf{u} = (u_1, u_2)$ (a scalar!) can also be written as:

$$D_{\mathbf{u}} f(x_1, x_2) = \nabla f \cdot \vec{\mathbf{u}} = |\nabla f| |\vec{\mathbf{u}}| \cos \beta = |\nabla f| \cos \beta$$

- Where β is the angle between \mathbf{u} and ∇f
- However, $\cos \beta \leq 1$.
- Therefore:
 1. The greatest increase in the function happens in the direction of the gradient (i.e. $\beta = 0$)
 2. The greatest decrease is in the direction $-\nabla f$ (i.e $\beta = 180^\circ$)

Steepest ascent and Iso-Contours

- Steepest ascent follows the gradient direction
- Using same argument, when the direction u is perpendicular to the gradient, $\cos\beta = 0$ and there is no change in the function – this is exactly the direction of the iso-contours, walking with no change in altitude.



The gradient of n-dimensional functions

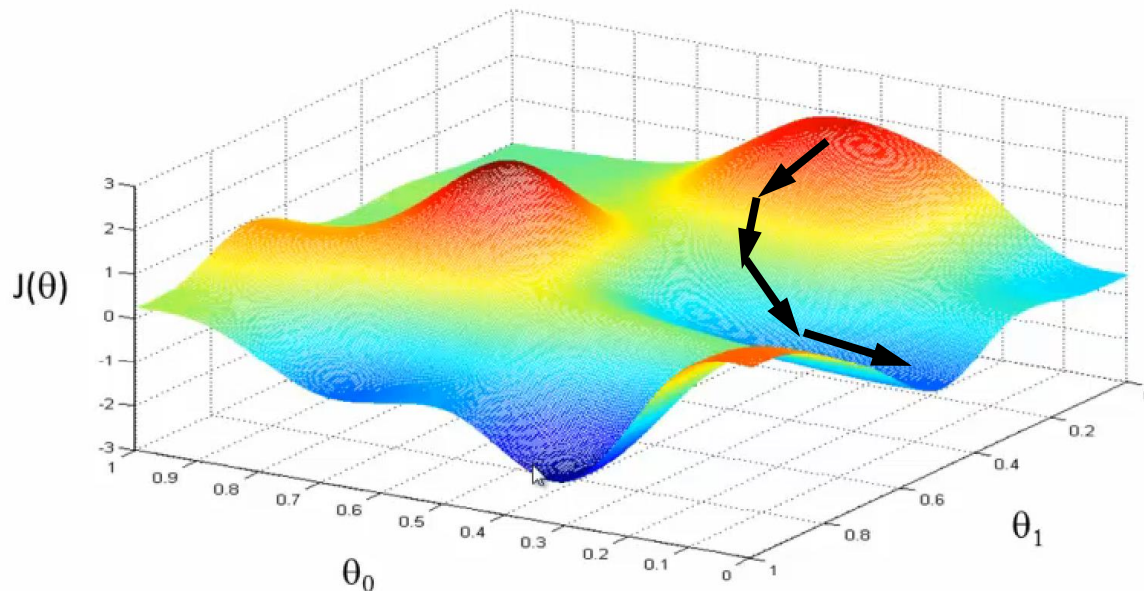
- For an n-D function $y = f(x_1, x_2, \dots, x_n)$ the gradient is defined as :

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right)$$

- The gradient vector at any given point is the direction of greatest increase of f at this point.
- The direction of greatest decrease of f is opposite to the gradient: $-\nabla f(x_1, x_2 \dots x_n)$

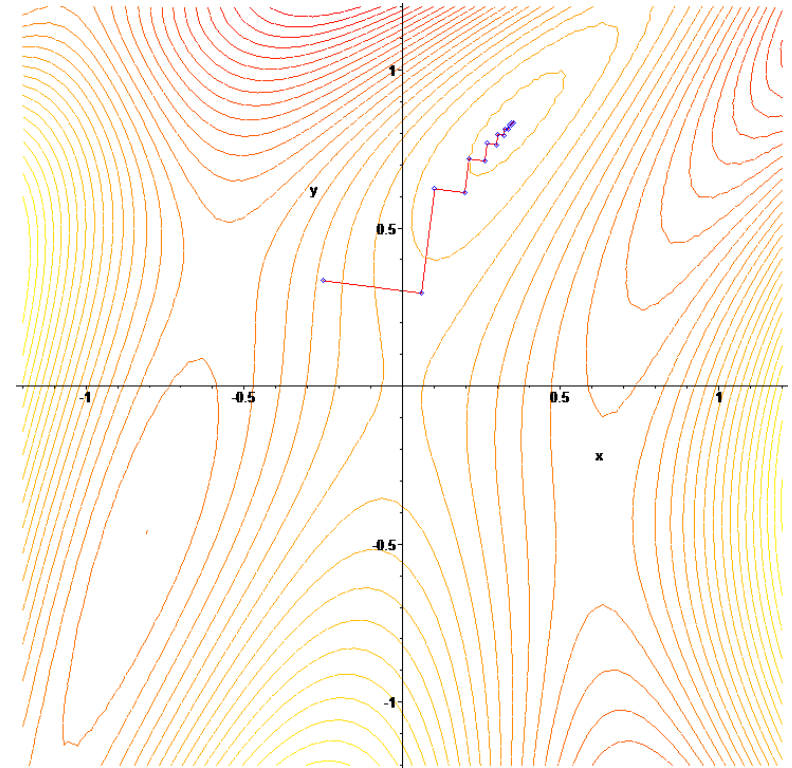
How to find a minimum of a (reasonably smooth) n-dimensional function?

- Take steps in the direction of maximum decrease – i.e. opposite the gradient direction!
- This is called **Gradient Descent**



Gradient Descent Steps

- For a small enough $\alpha > 0$ we have
$$f(x - \alpha \nabla f(x)) < f(x),$$
so we take one step of size α in the opposite direction of the gradient.
- This represents greedy local descent
- Note:
such steps can zig-zag



Back to Minimizing the Cost Function in Linear Regression

- Recall that our best model, θ^* , is the one that minimizes the cost function. That is:

$$\theta^* \text{ attains } \min_{\theta} [J(\theta)] = \min_{\theta} \left[\frac{1}{2m} \sum_{i=1}^m (\theta \cdot \mathbf{x}^{(i)} - y^{(i)})^2 \right]$$

- $J(\vec{\theta})$ is a real valued function of $\vec{\theta} \in \mathbb{R}^n$
- So - we can start with some initial guess $\vec{\theta}_0^*$ and then use gradient descent

Gradient Descent Algorithm

- Start with some value $\theta(0) = (\theta_0, \theta_1, \theta_2, \dots, \theta_n)$
- Repeat until you reach a minimum:
 - For all $j = 0 \dots n$,
 - Update $\theta_j(t + 1) \leftarrow \theta_j(t) - \alpha \frac{\partial}{\partial \theta_j} J(\theta(t))$
- $\alpha > 0$ is a parameter of the algorithm called the learning rate
- Updates are simultaneous (in all $n + 1$ directions)
- In the general case this process can still be trapped in local minima!

Minimizing the Cost Function

- This gradient descent process is seeking:

$$\boldsymbol{\theta}^* = \arg \min_{\boldsymbol{\theta}} [J(\boldsymbol{\theta})] = \arg \min_{\boldsymbol{\theta}} \left[\frac{1}{2m} \sum_{i=1}^m (\boldsymbol{\theta} \cdot \mathbf{x}^{(i)} - y^{(i)})^2 \right]$$

- Missing details?

Calculating the Partial Derivatives

$$\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1, \dots, \theta_n) = \frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$= \frac{1}{2m} \sum_{i=1}^m \frac{\partial}{\partial \theta_j} (\theta_0 + \theta_1 x_1^{(i)} + \dots + \theta_j x_j^{(i)} + \dots + \theta_n x_n^{(i)} - y^{(i)})^2$$

$$= \frac{1}{2m} \sum_{i=1}^m 2(\theta_0 + \theta_1 x_1^{(i)} + \dots + \theta_j x_j^{(i)} + \dots + \theta_n x_n^{(i)} - y^{(i)}) \cdot x_j^{(i)}$$

$$= \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)}$$

Gradient Descent for Linear Regression

- Initialize $\theta = (\theta_0, \theta_1, \theta_2, \dots, \theta_n)$
- Repeat until you reach a minimum (or stop cdn):
 - For all $0 \leq j \leq n$,

$$\theta_j(t+1) = \theta_j(t) - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta(t)}(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)}$$

- In words: set the new θ_j to the current θ_j minus the learning rate (α) times the partial derivative of the error function with respect to θ_j , computed at the current θ .
- Also remember that $x_0^{(i)} = 1$

Closed form solution?

$$X \cdot \theta = y$$

$$\begin{matrix} & & n+1 & & \theta \in \mathbb{R}^{n+1} & & Y \in \mathbb{R}^m \\ m & \begin{pmatrix} x_0^{(1)} & x_1^{(1)} & \dots & x_n^{(1)} \\ x_0^{(2)} & x_1^{(2)} & \dots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_0^{(m)} & x_1^{(m)} & \dots & x_n^{(m)} \end{pmatrix} & \begin{pmatrix} \theta_0 \\ \vdots \\ \theta_n \end{pmatrix} & = & \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{pmatrix} \end{matrix}$$

- If X is square and non singular we can write $\vec{\theta} = X^{-1}y$
- In ML typically X is overdetermined ($m \gg n$).

Recitation

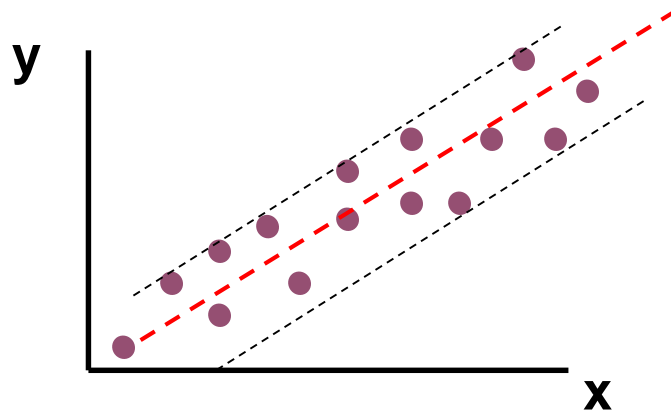
- Description of HWA1
- Feature scaling
- Learning rate
- Python

Extra slides/notes

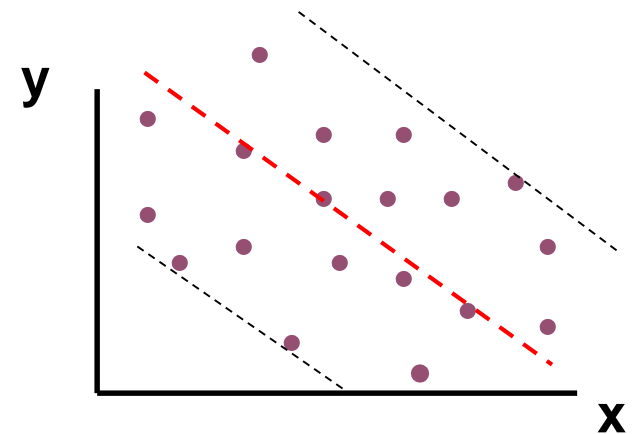
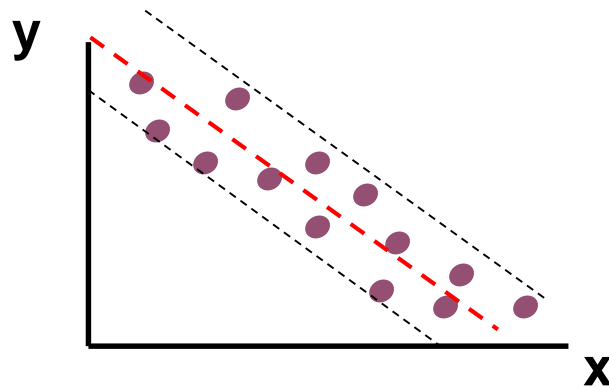
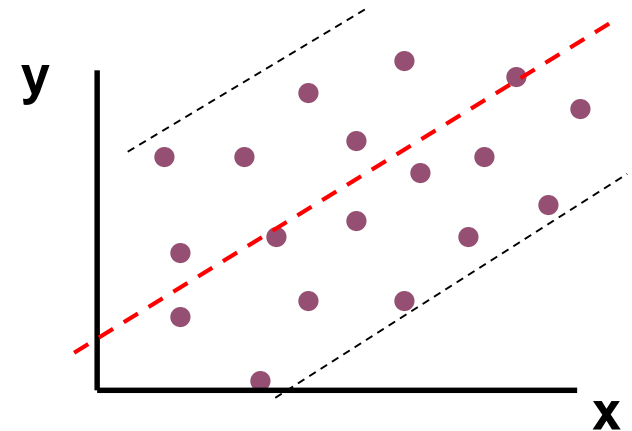
- Correlations
- Pseudo-inverse of a matrix (closed form solution)
- Going beyond Linear (also in the HW)

Strong vs. Weak Linear Relationship

Strong relationships

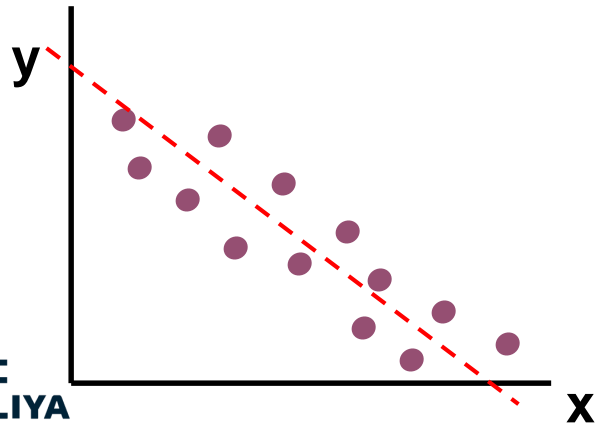
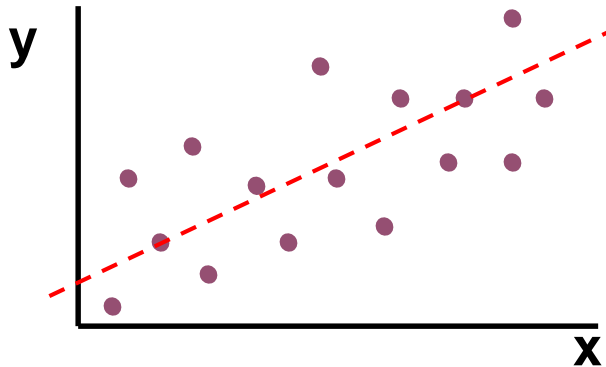


Weak relationships

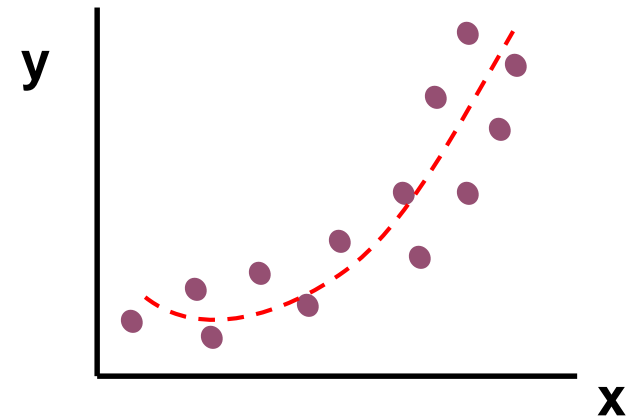
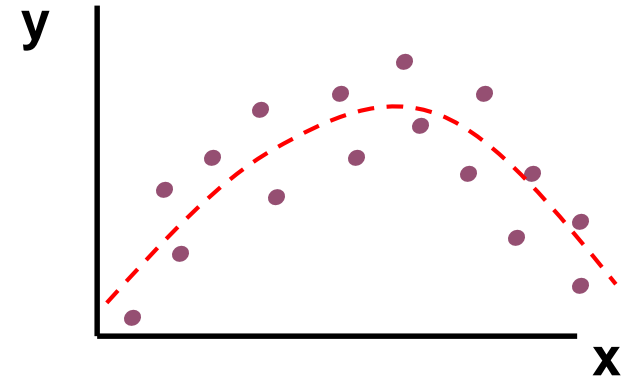


Not Everything is Linear!

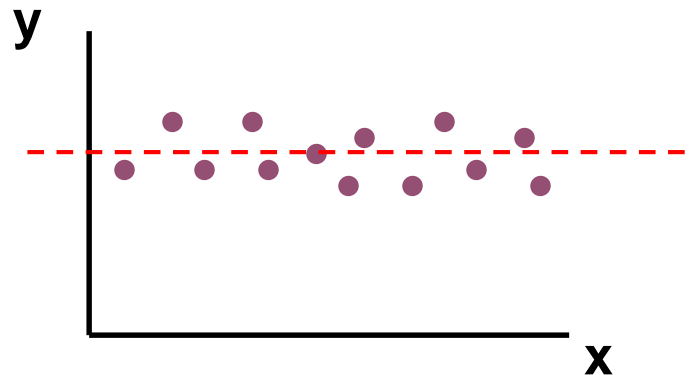
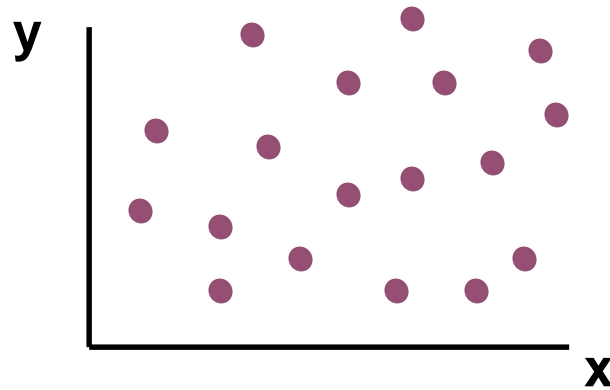
Linear relationships



Curvilinear relationships



No Evident Relationship



Correlation Analysis

- **Correlation** analysis is used to measure strength of the association (**linear relationship**) between two variables
 - Only concerned with strength of the relationship
 - No causal effect is implied
- The **sample (Pearson) correlation coefficient r** is a measure of the strength of the linear relationship between two variables, based on sample observations

The Pearson Correlation Coefficient

$$r = \frac{\sum_{i=1}^m (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^m (x_i - \bar{x})^2 \sum_{i=1}^m (y_i - \bar{y})^2}} = \frac{\sigma_{xy}}{\sigma_x \sigma_y}$$

Where:

r = Sample Pearson correlation coefficient

m = Number of samples

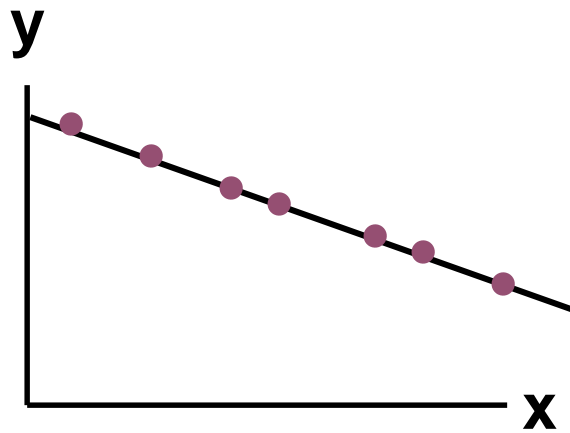
x = Value of an explaining variable

y = Value of the dependent variable

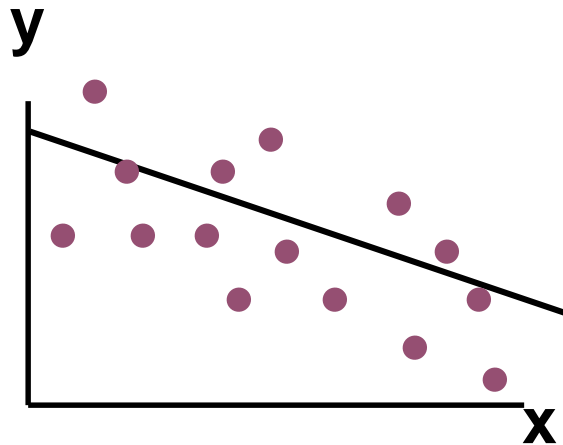
Features of r

- Unit free
- Ranges between -1 and 1
- The closer to 0, the weaker the linear relationship
- The closer to -1, the stronger the negative linear relationship
- The closer to 1, the stronger the positive linear relationship

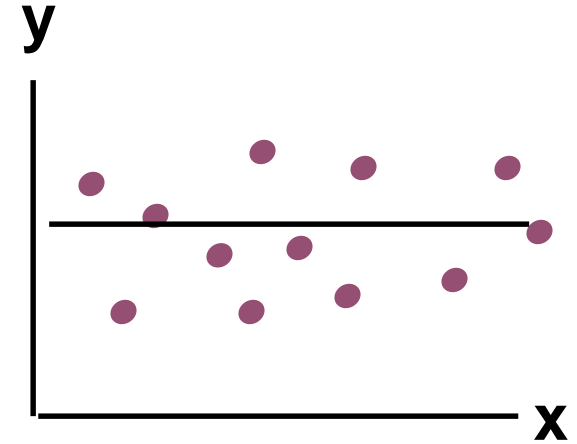
Examples of r Values



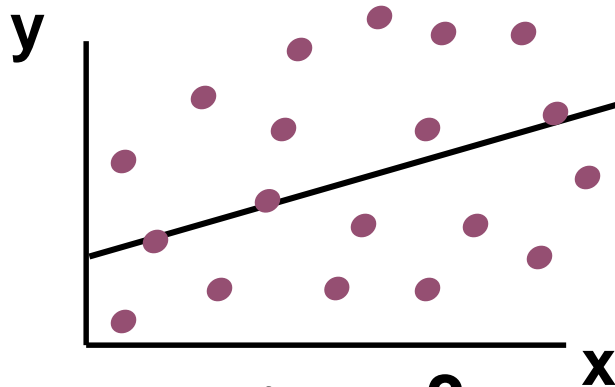
$r = -1$



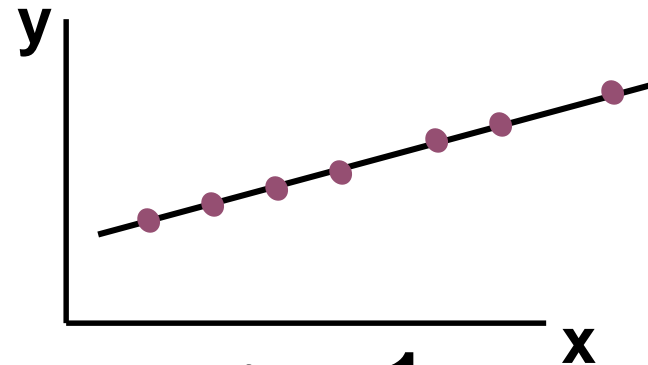
$r = -.6$



$r = 0$

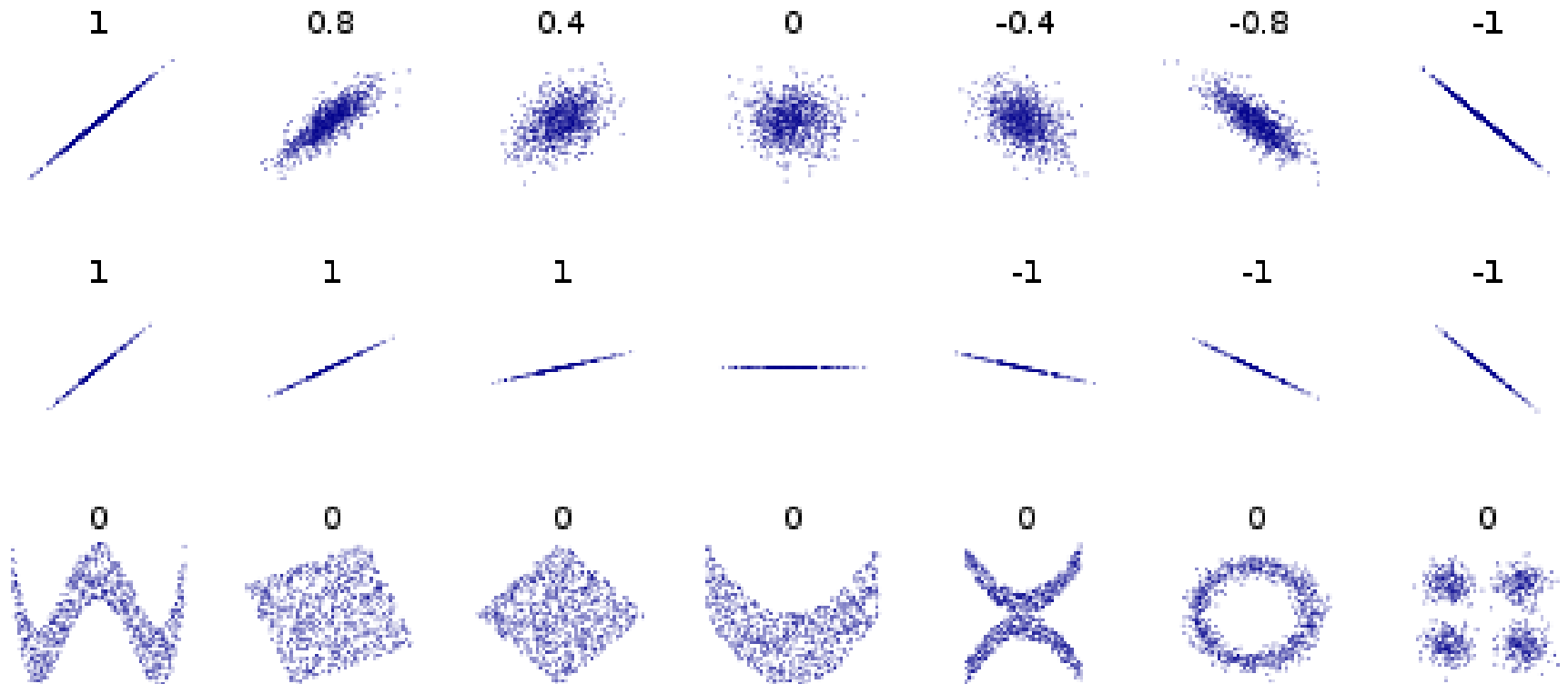


$r = +.3$



$r = +1$

More Complex Relationships May Not Be Captured Using Pearson r



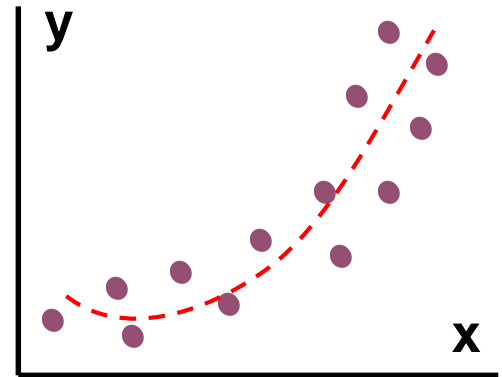
Polynomial Regression

- We can expand our feature space by using functions of the original features.
- For example, if we want to use a cubic function feature space we can define:

$$x_0 = 1, x_1 = x, x_2 = x^2, x_3 = x^3$$

then use regular regression and in essence we are learning the function

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$



Other Functions

- We can use other functions of features such as $x^{1/q}$
- We can define functions of sets of variables such as $x_1x_5x_7$ or $x_1^2x_5x_7^3$
- All of these can be represented as new features and increase the dimension of the entire calculation

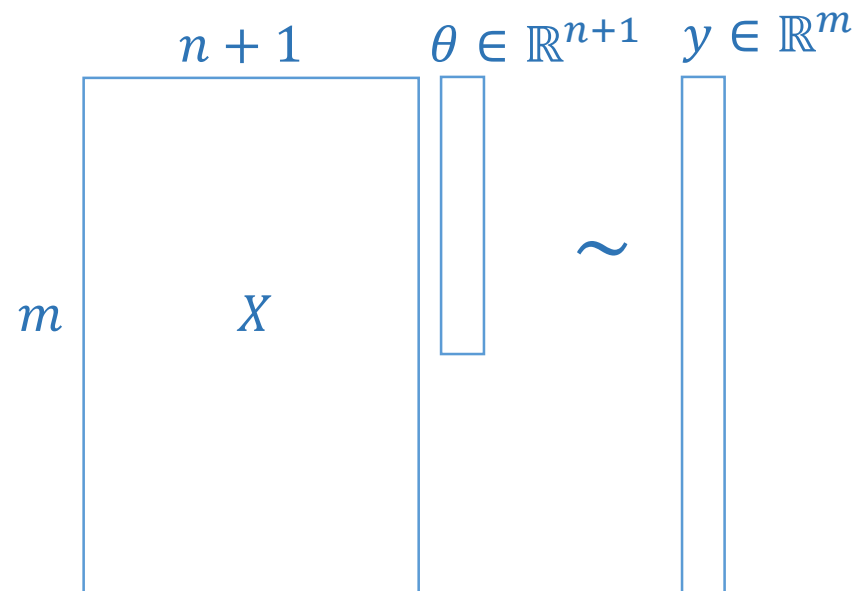
Closed form solution?

$$X \cdot \theta = y$$

$$\begin{matrix} & & n+1 & & \theta \in \mathbb{R}^{n+1} & & Y \in \mathbb{R}^m \\ m & \begin{pmatrix} x_0^{(1)} & x_1^{(1)} & \dots & x_n^{(1)} \\ x_0^{(2)} & x_1^{(2)} & & x_n^{(2)} \\ & \vdots & \ddots & \vdots \\ x_0^{(m)} & x_1^{(m)} & \dots & x_n^{(m)} \end{pmatrix} & \begin{pmatrix} \theta_0 \\ \vdots \\ \theta_n \end{pmatrix} & = & \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{pmatrix} \end{matrix}$$

- If X is square and non singular we can write $\vec{\theta} = X^{-1}y$
- Most of the time X is overdetermined ($m \gg n$).

Schematic set-up



Minimum when $\nabla = 0$

- Remember the (MSE) cost function:

$$E(\boldsymbol{\theta}) = \|X \cdot \vec{\boldsymbol{\theta}} - \mathbf{y}\|_2^2 = \sum_{i=1}^m (x^{(i)} \boldsymbol{\theta}^T - y^{(i)})^2$$

- This will be minimal when the gradient ∇E is 0.
- Forming the derivatives yields (see below):

$$\nabla E(\boldsymbol{\theta}) = \sum_{i=1}^m 2(x^{(i)} \boldsymbol{\theta}^T - y^{(i)}) x^{(i)} = 2X^T(X\boldsymbol{\theta} - \mathbf{y})$$

Proof

$$\nabla E(\theta) = 0, \quad \nabla E(\theta) = \left(\frac{\partial E}{\partial \theta_j}(\theta) \right)_{j=1}^n$$

Expanding the partial derivatives, we get the following expression (for setting to 0)

$$(\nabla E(\theta))_j = \frac{\partial E}{\partial \theta_j}(\theta) = \frac{\partial}{\partial \theta_j} \left(\sum_{i=1}^m (X(i, :) \cdot \theta - y(i))^2 \right)$$

Recall that $X(i, :)$ is the notation for the i^{th} row. Now we expand the dot product

$$\begin{aligned} \frac{\partial E}{\partial \theta_j}(\theta) &= \frac{\partial}{\partial \theta_j} \left(\sum_{i=1}^m \left(\left(\sum_{k=1}^n X(i, k) \cdot \theta_k \right) - y(i) \right)^2 \right) \\ \frac{\partial E}{\partial \theta_j}(\theta) &= \left(\sum_{i=1}^m \frac{\partial}{\partial \theta_j} \left(\left(\sum_{k=1}^n X(i, k) \cdot \theta_k \right) - y(i) \right)^2 \right) \\ \frac{\partial E}{\partial \theta_j}(\theta) &= \left(\sum_{i=1}^m 2 \left(\left(\sum_{k=1}^n X(i, k) \cdot \theta_k \right) - y(i) \right) \cdot X(i, j) \right) \end{aligned}$$

Proof, cont

For all $j \neq k$ the derivative is 0, so we only consider θ_j

$$\nabla E(\theta) = \left(2 \sum_{i=1}^m (X(i, :) \cdot \theta - y(i)) \cdot X(i, j) \right)$$
$$\nabla E(\theta) = (2X(:, j)(X \cdot \theta - y))$$

Notice that $(X(:, j))^T = X^T(j, :)$ and therefore

$$\nabla E(\theta) = (2X^T(j, :)(X \cdot \theta - y))$$
$$\nabla E(\theta) = (2X^T(X \cdot \theta - y))$$

Recall that we want to solve for the θ that makes this 0:

$$0 = 2X^T(X \cdot \theta - y)$$
$$0 = (X^T X \cdot \theta - X^T y)$$
$$X^T X \cdot \theta = X^T y$$
$$\theta = (X^T X)^{-1} X^T y$$

Pseudo-inverse & the closed form solution - Summary

- Setting the gradient of E to zero yields the necessary condition for minimum (see notes and slides above): $X^T X \cdot \theta = X^T y$
- Now, $X^T X$ is square and often nonsingular and so we can solve for θ uniquely as:

$$\theta = \text{pinv}(X)y \quad \text{where} \quad \text{pinv}(X) = (X^T X)^{-1} X^T$$

- The $n \times m$ matrix $\text{pinv}(X) = (X^T X)^{-1} X^T$ is called the **pseudo inverse** of X (which is $m \times n$)
- If X is square it is just its inverse.

Gradient Descent and Pseudo Inverse

- $X^T X$ can still be singular (or not full rank) and not have an inverse. This can be resolved with some more algebra.
- This pinv technique doesn't work for all error functions J . Gradient descent is more general.
- Gradient descent allows parallelization.

Summary

- Regression learns a function to predict values based on a vector of features
- Linear Regression uses a Gradient Descent Algorithm or a Pseudo-Inverse solution
- Gradient descent is a general minimization procedure
- There are other (non-linear) relations between variables
- The Pearson correlation coefficient is a measure of the strength of the linear relationship between two variables
- Pseudo inverse solution

Summary - cont

The execution algorithm:
 $y = f(x) = x\theta^T$

