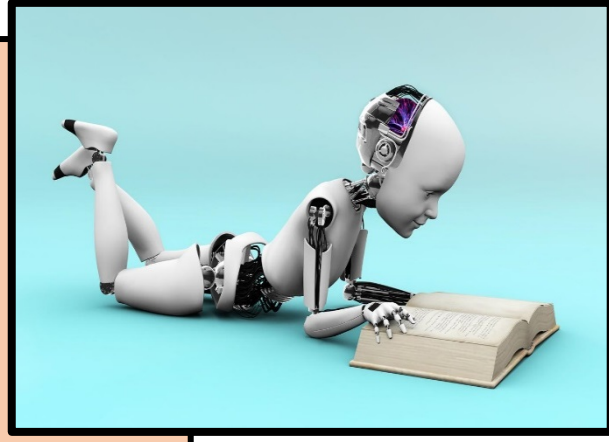
Machine learning from data
Class1: Linear Regression



Zohar Yakhini

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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

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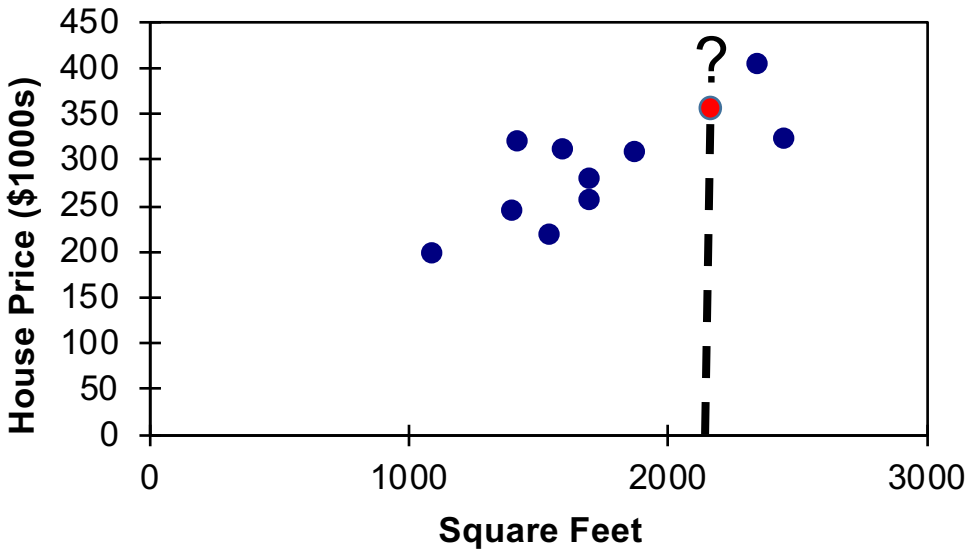
Statistics:
Dependent variable (y) = house price
Explaining variable (x) = square footage

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)?

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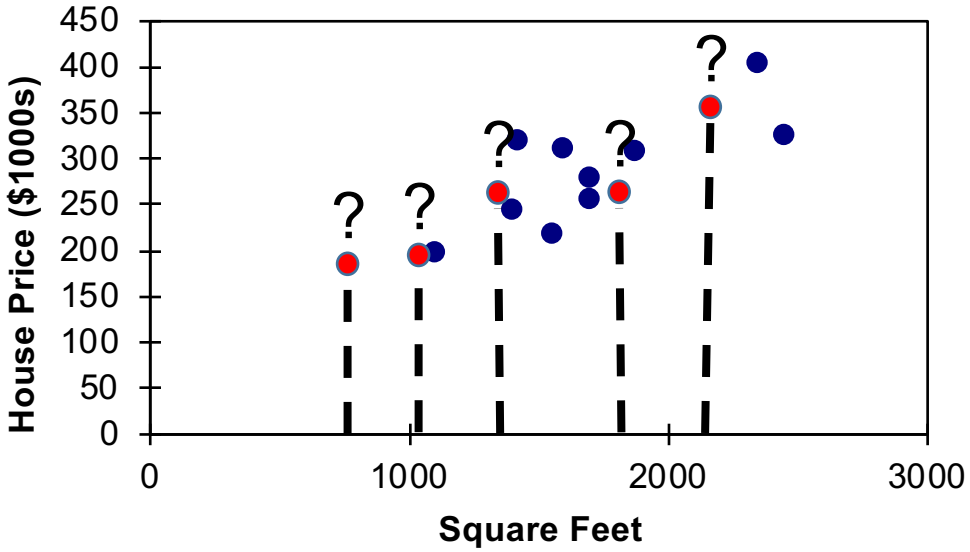
Memorization?



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

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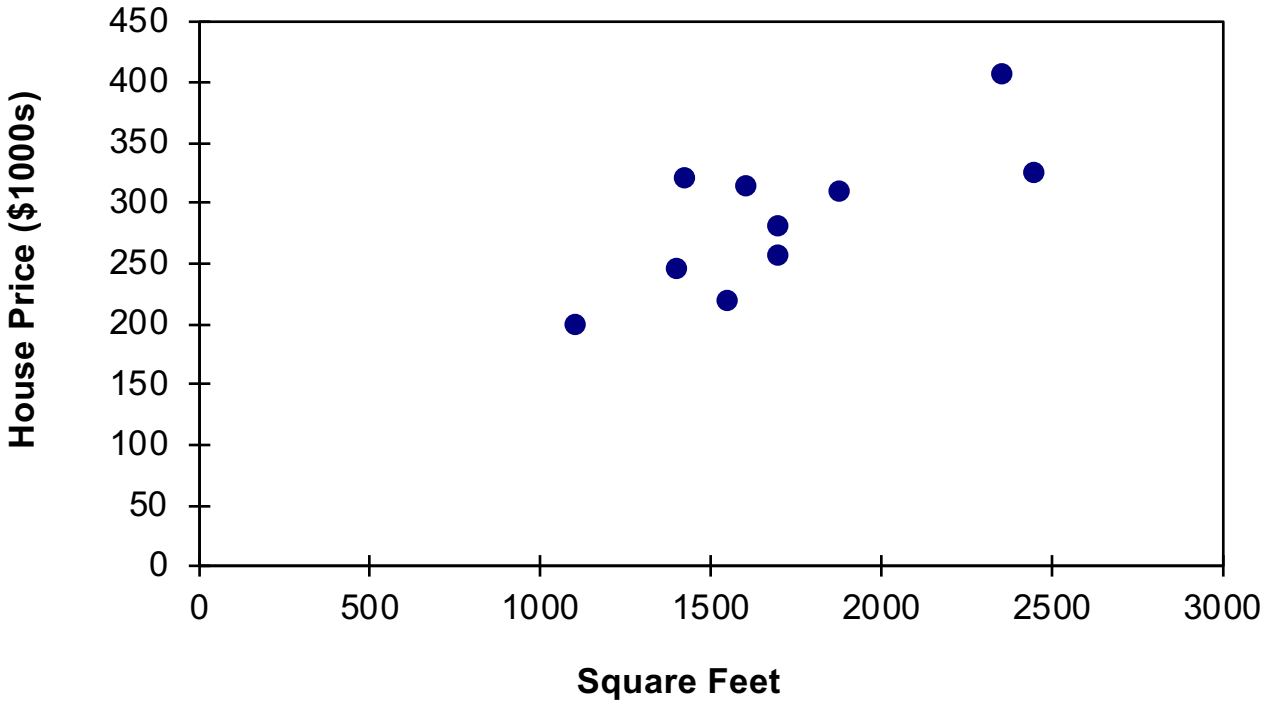
OK … a function?



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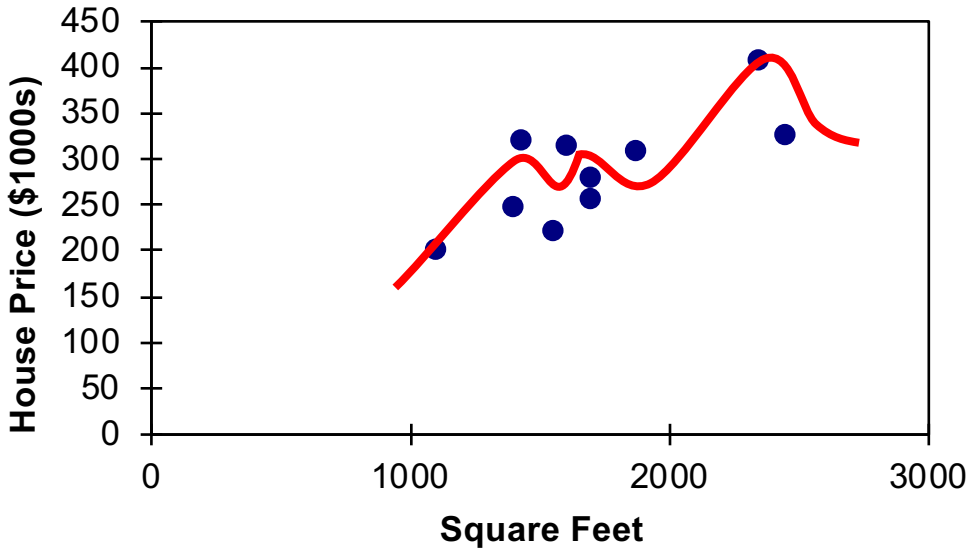
Generalization: Learn a Function



But which function y=f(x)?

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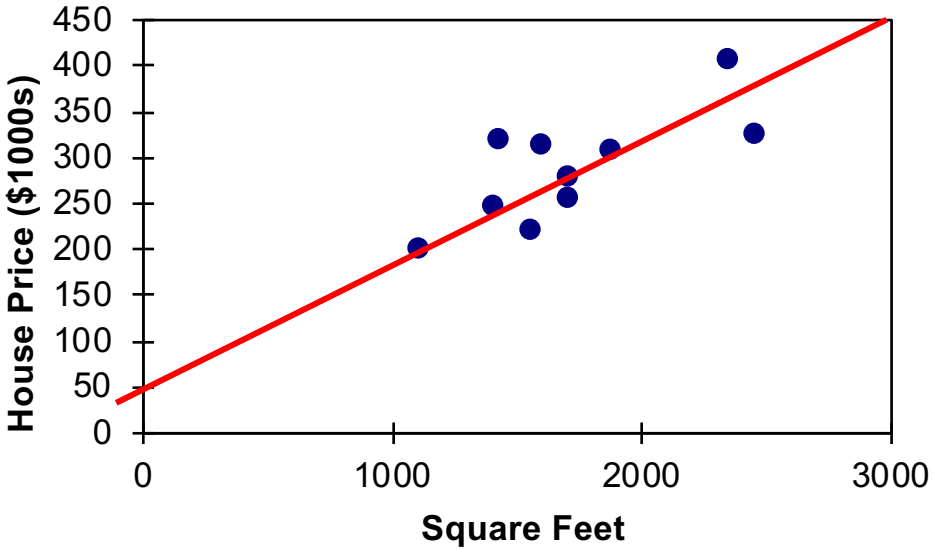
Simplest: Linear Model



- 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

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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…

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Multiple Features

- Let $\mathbf{x^{(i)}} = \left(\mathrm{x}_1^{(i)}, \mathrm{x}_2^{(i)}, \ldots, \mathrm{x}_n^{(i)}\right)$

  be the vector of feature values for each instance i
- For simplicity we add another "constant" feature for every i

$$\mathrm{x}_0^{(i)} = 1$$

- For n features our linear hypothesis will be represented by the parameters $\boldsymbol{\theta} = \left(\theta_0, \theta_1, \theta_2, \ldots, \theta_n\right)$

  for which we have:

$$\mathrm{y} = \theta_0 + \theta_1 \mathrm{x}_1 + \theta_2 \mathrm{x}_2 + \cdots + \theta_\mathrm{n} \mathrm{x}_\mathrm{n}$$

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

  is the vector of parameters that defines our function (or our **model**)

The Hypothesis (or model) is the execution algorithm

- How does a specific set of values,

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

  which defines a specific hypothesis (model) help us?
- How can we use it?
- Given a new house instance $\mathbf{x}' = (\mathrm{x}'_0, \mathrm{x}'_1, \ldots, \mathrm{x}'_n)$ we can estimate its price by an inner product with the vector $\boldsymbol{\theta}$:

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

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Finding the Best Hypothesis/Model

- There are many possible parameter vectors

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

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 $\mathbf{x^{(i)}} = \left(\mathrm{x}_0^{(i)}, \mathrm{x}_1^{(i)}, \ldots, \mathrm{x}_n^{(i)}\right)$

as well as the value $\mathrm{y}^{(i)}$

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"Training" or "Learning"

- 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 $\boldsymbol{\theta}$ such that <u>for all</u> instances i in the training set we will have:

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

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

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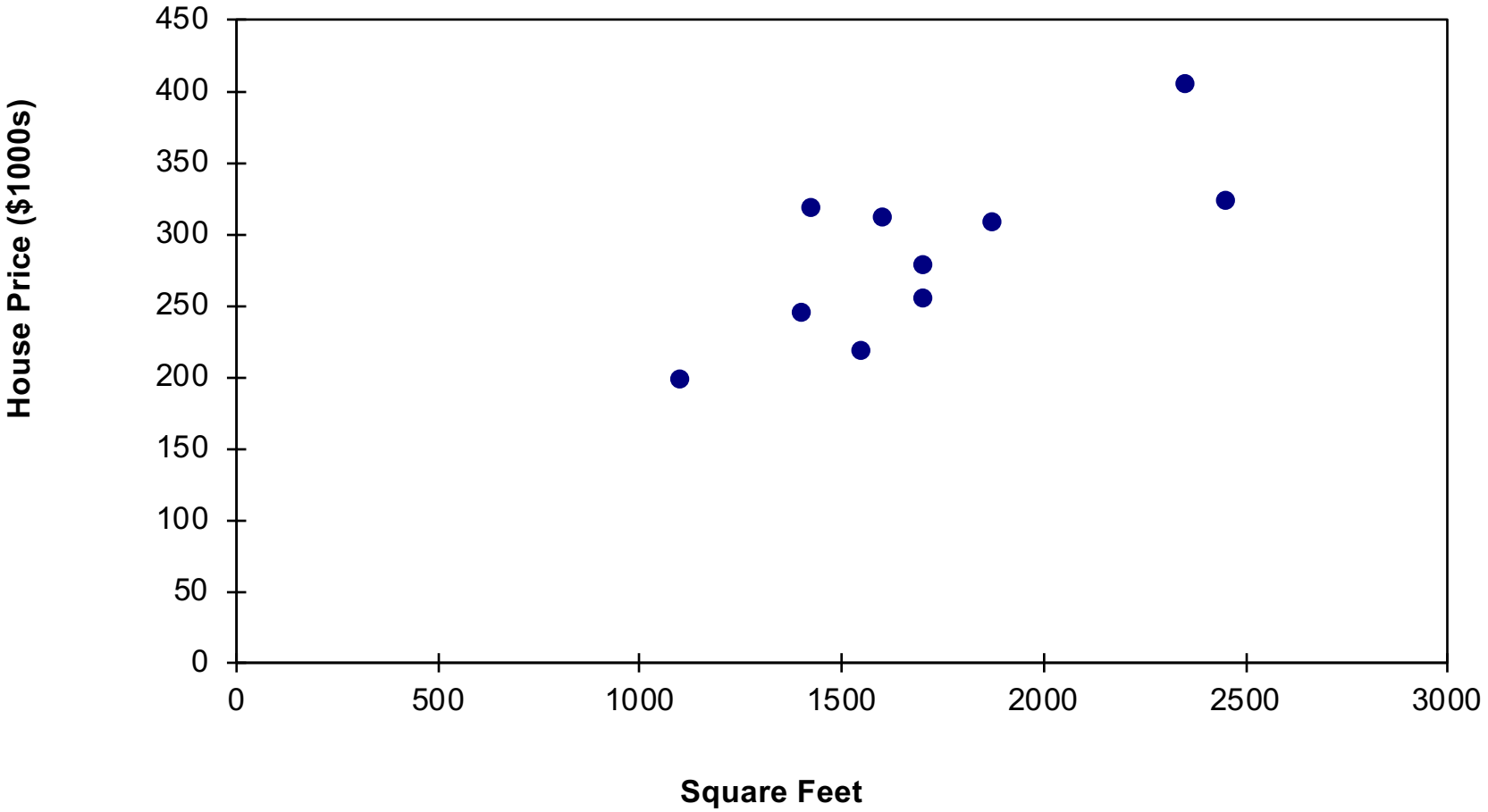

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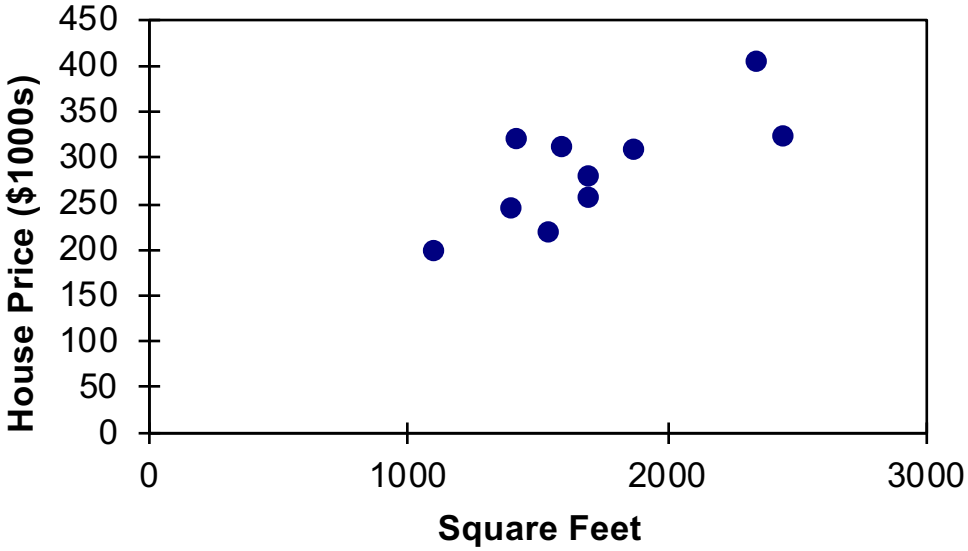
Consistent Learners

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



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Cost Function of a Model θ

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

Prediction *Actual value*

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

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

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

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

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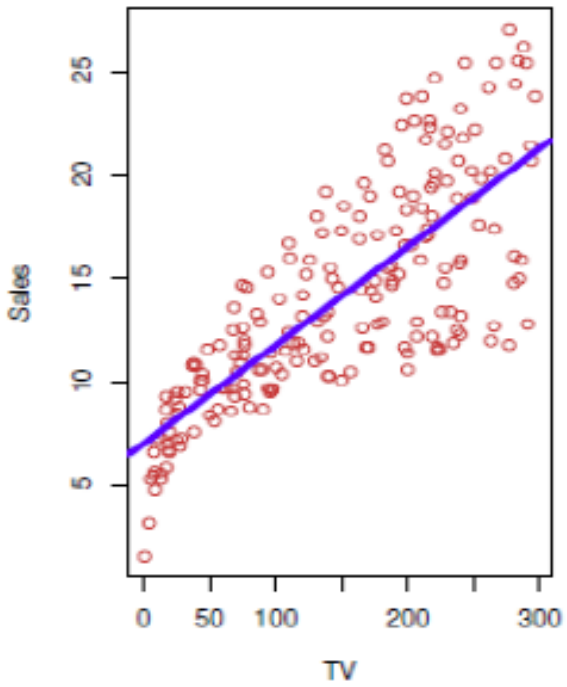
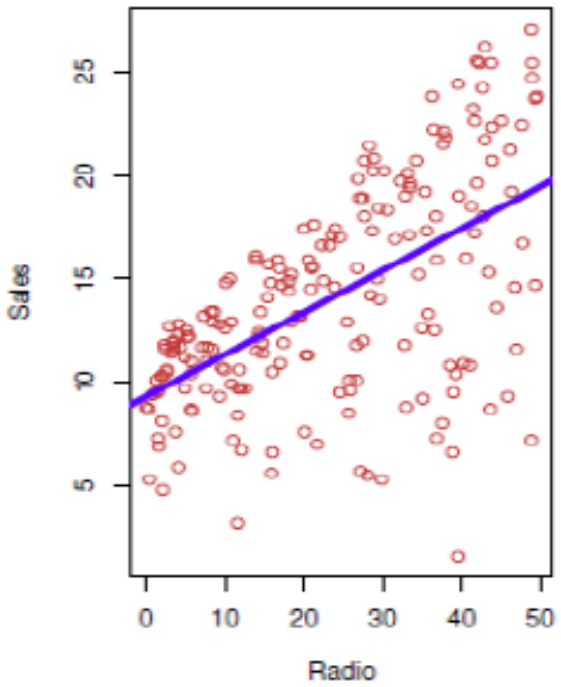
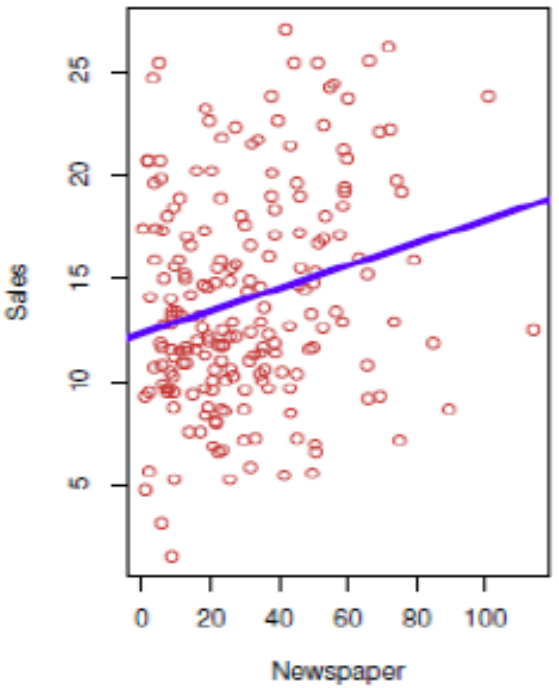
Example: advertising and sales







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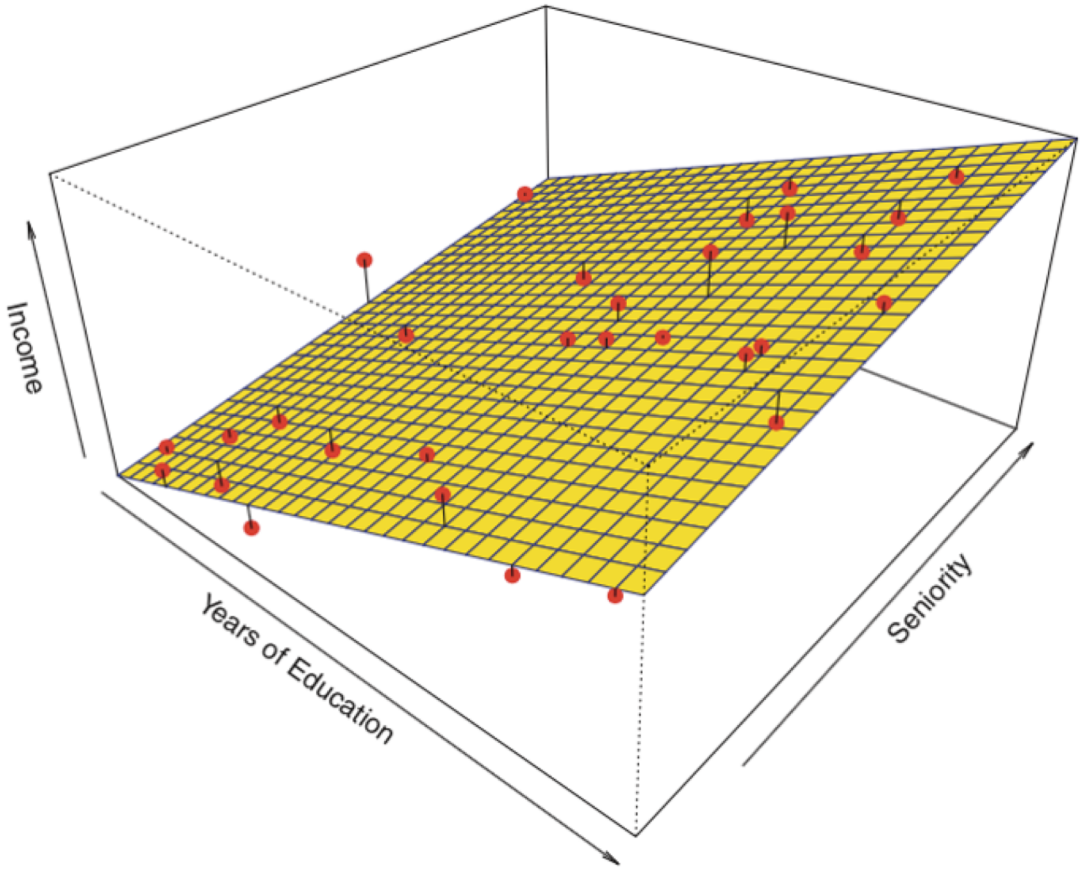
In higher dimensions



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Minimizing the Cost Function

- Hence, our best hypothesis $\boldsymbol{\theta}^*$ would be the one that minimizes the cost function:

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

- How can we find it?

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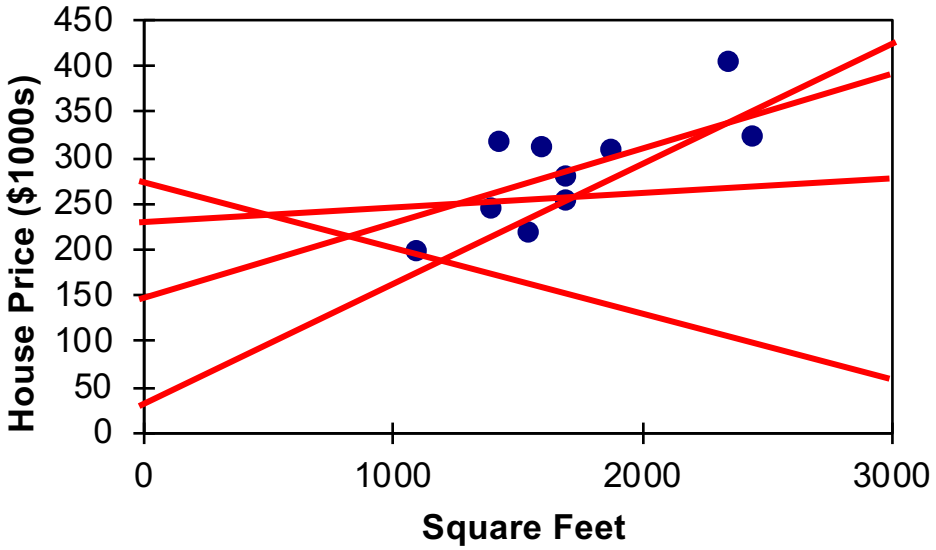
The Hypotheses Space

- 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)

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



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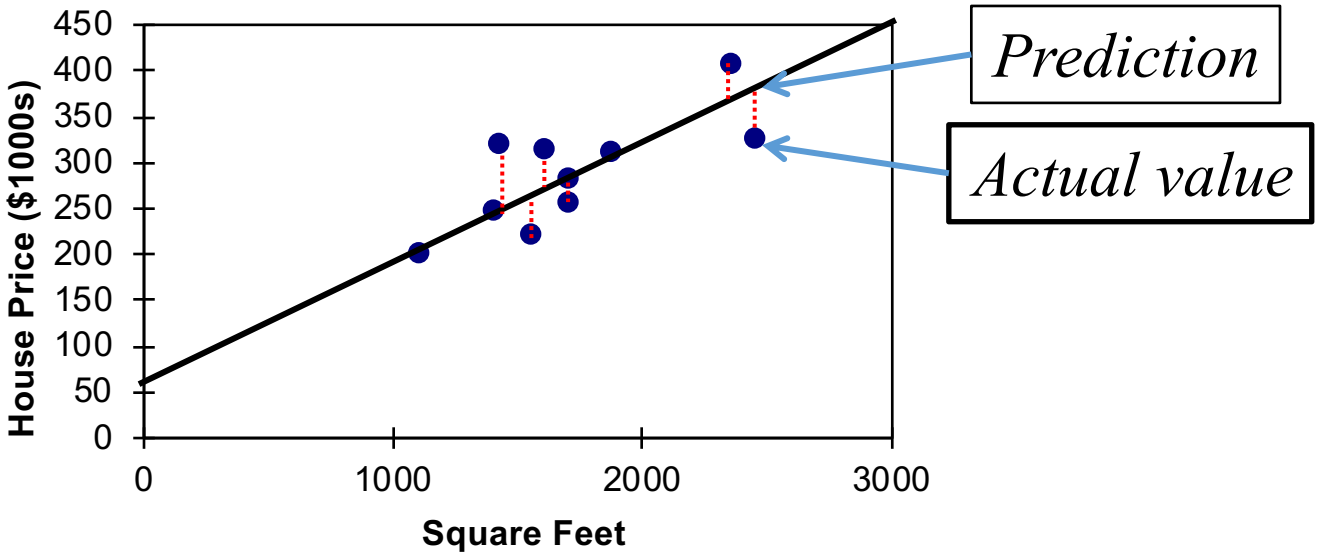
Geometric interpretation of the error

We search for θ_0 and θ_1 that minimize the sum of (squared) errors:

$$J(\boldsymbol{\theta}) = \frac{1}{2m}\sum_{i=1}^{m}\left(\theta_0 + \theta_1 x^{(i)} - y^{(i)}\right)^2$$



The Cost Function

θ_0, θ_1

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

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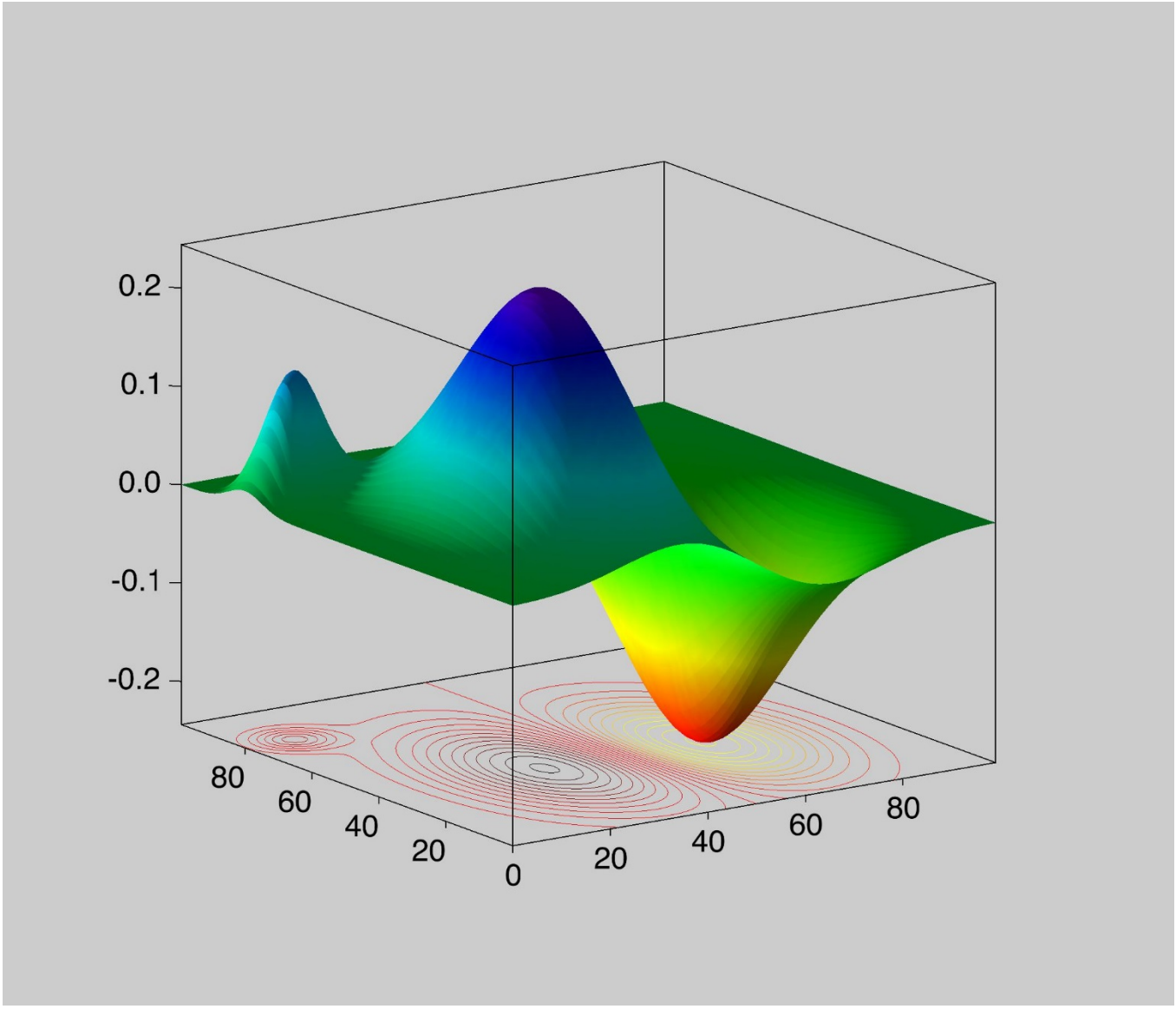
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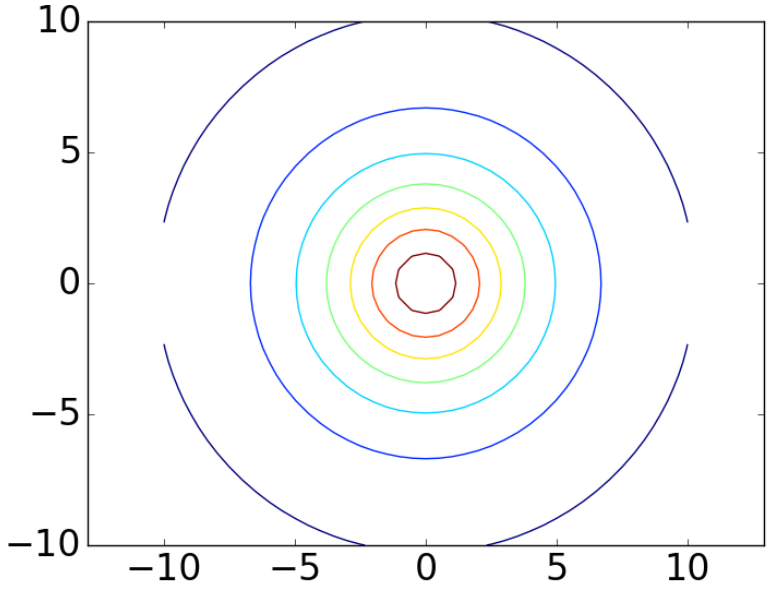
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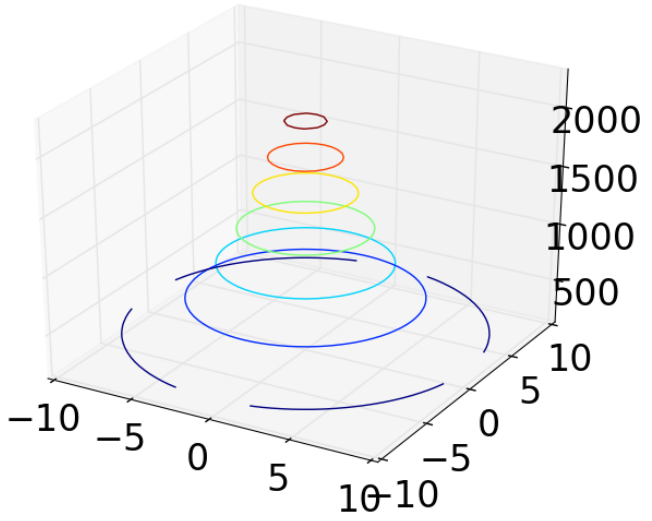
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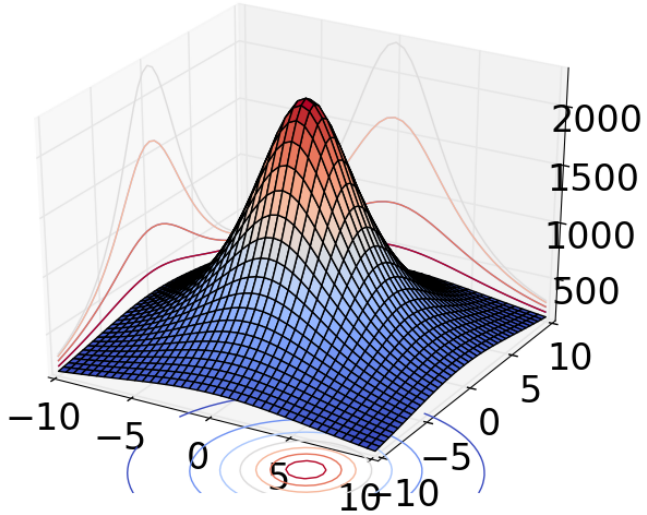
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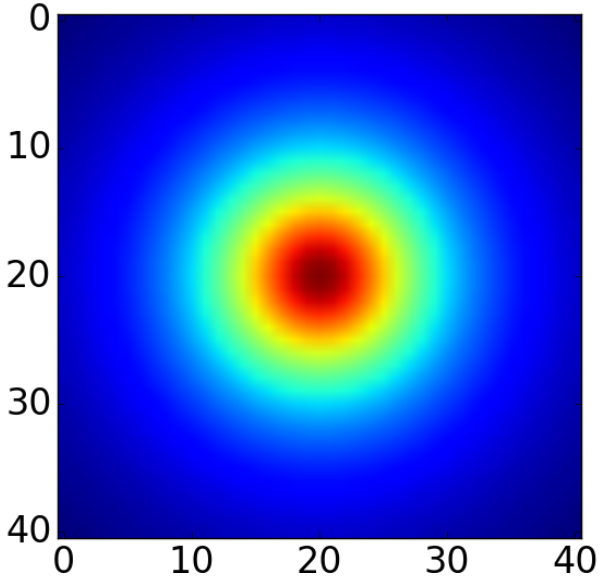
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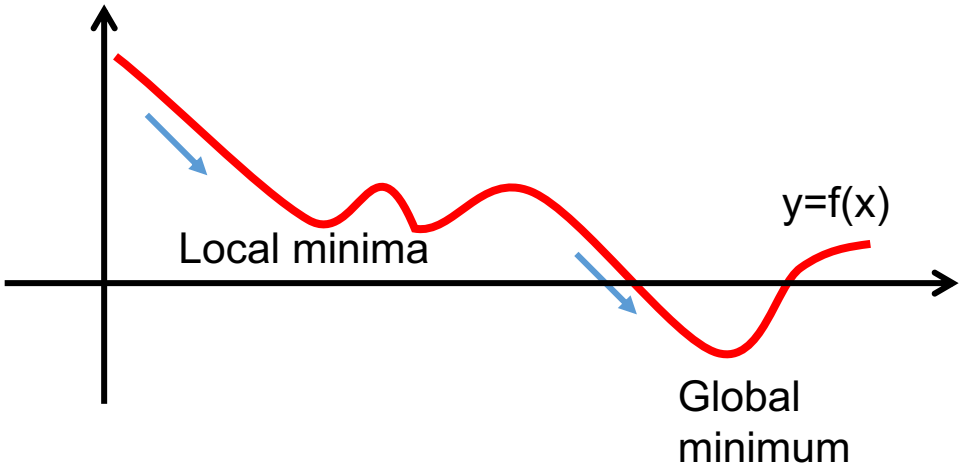
40
0
10
20
30
40

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 in the negative direction

- Can be trapped in local minimum!



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Directional Derivatives

- For a differentiable 2D function $f(x_1, x_2)$ the partial derivatives in the directions x_i are

$$\frac{\partial}{\partial x_1} f, \frac{\partial}{\partial x_2} f$$

- For example …

$$f(x, y) = 2x + 13y$$
$$f(x, y) = y \exp(x)$$
$$f(x, y) = 2x + 3xy + 5y^2$$

https://mathinsight.org/directional_derivative_gradient_introduction

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

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

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

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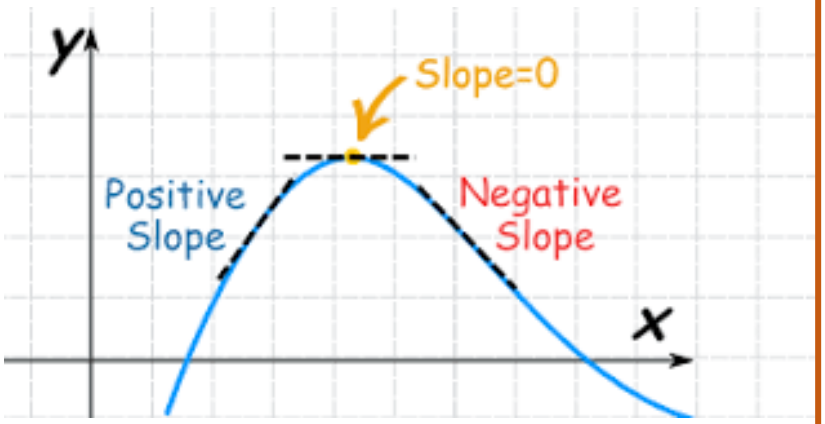
$$f(x,y) = y^4 e^x$$

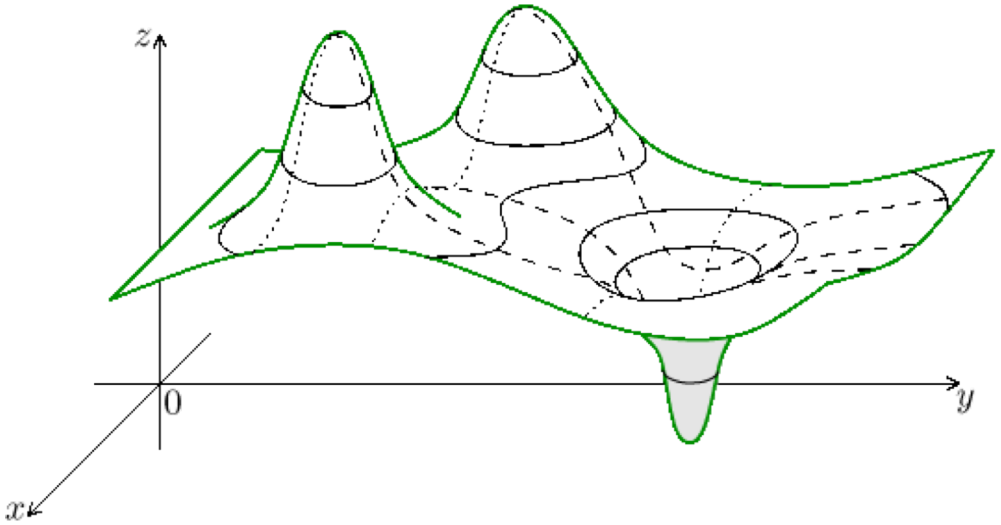
$$\frac{\partial f}{\partial x}(x,y) = y^4 e^x$$

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

Extrema and zero derivatives



1D



2D

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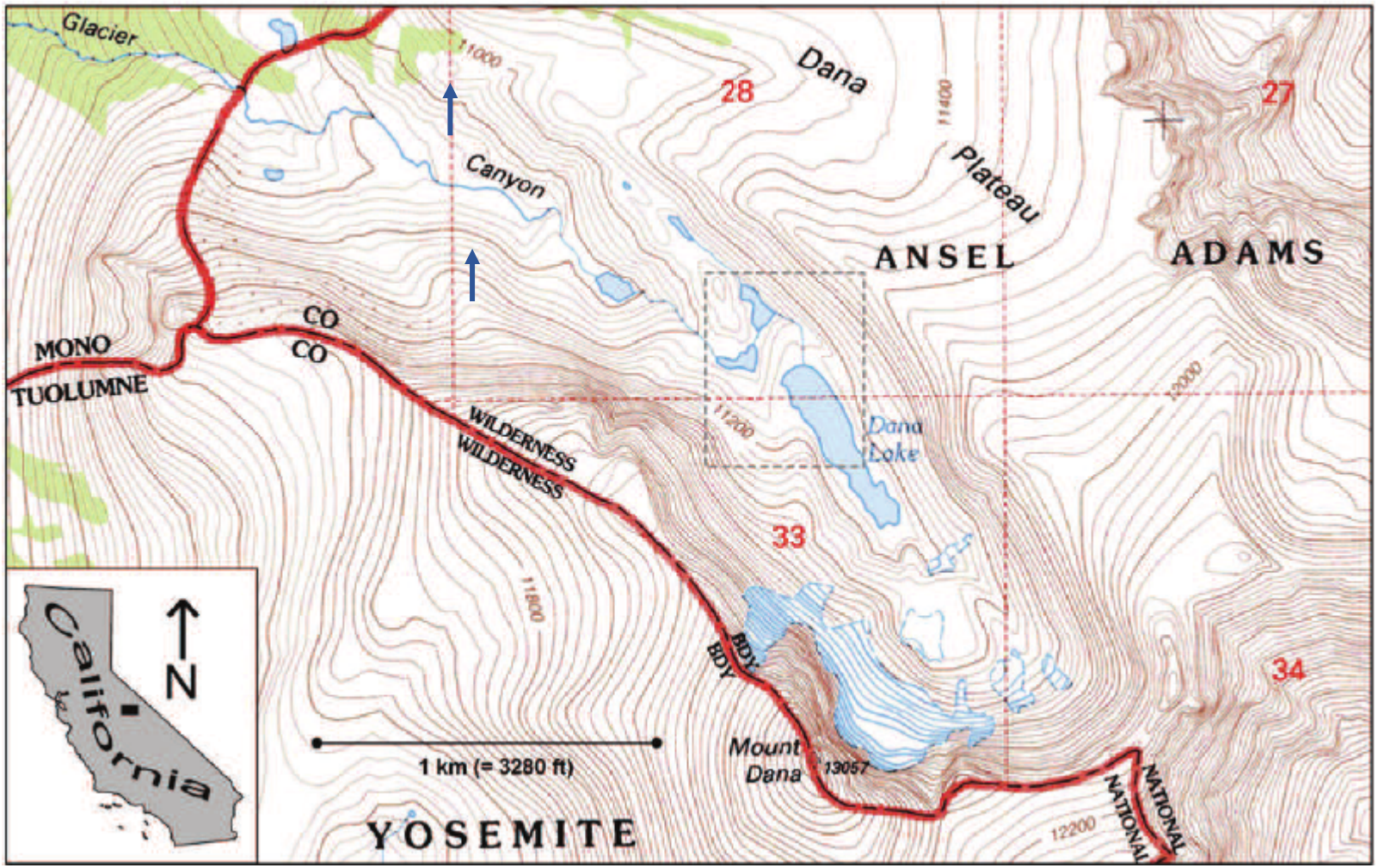
Example

What is the sign of the y directional derivative?



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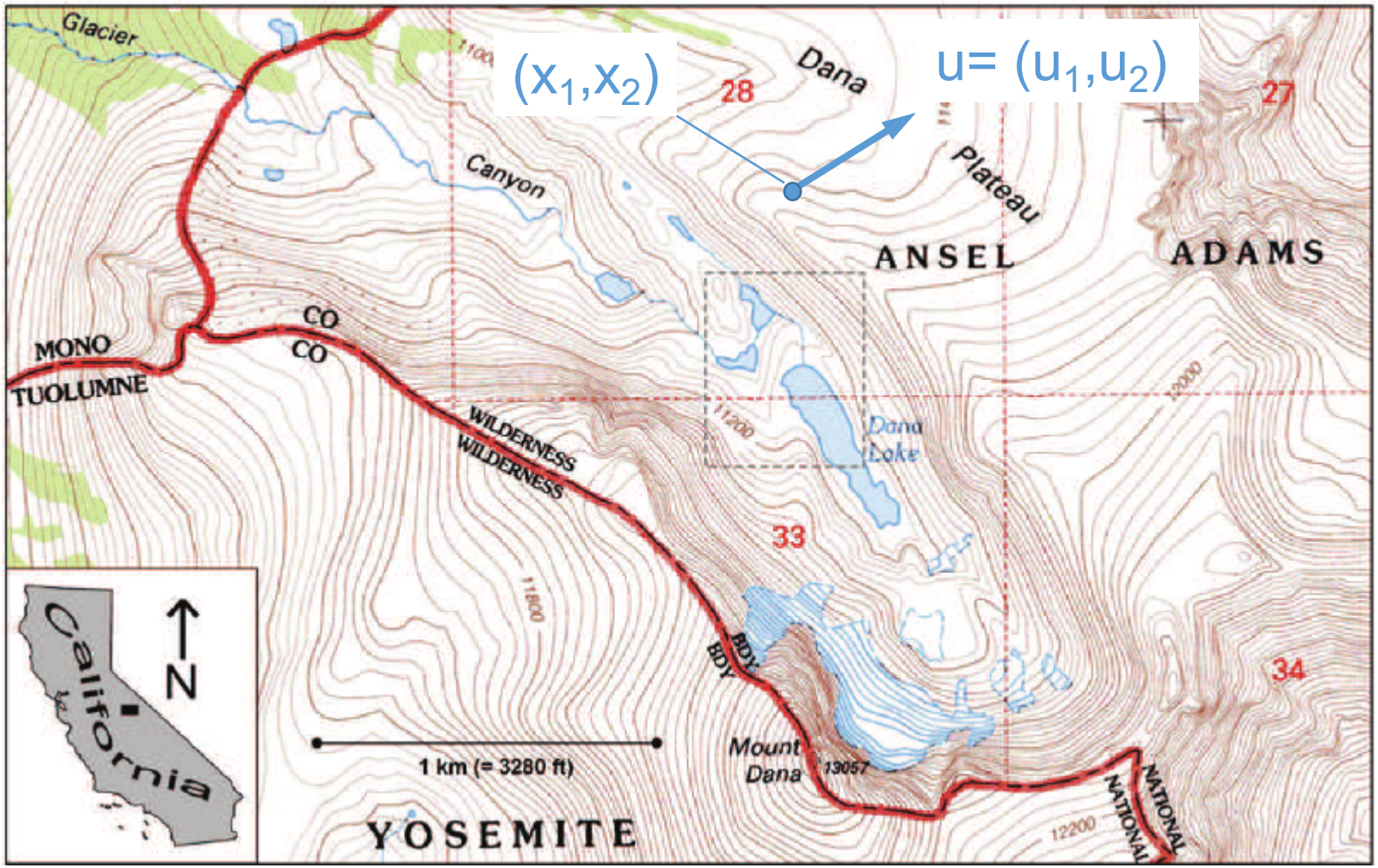
Example

Up or down?



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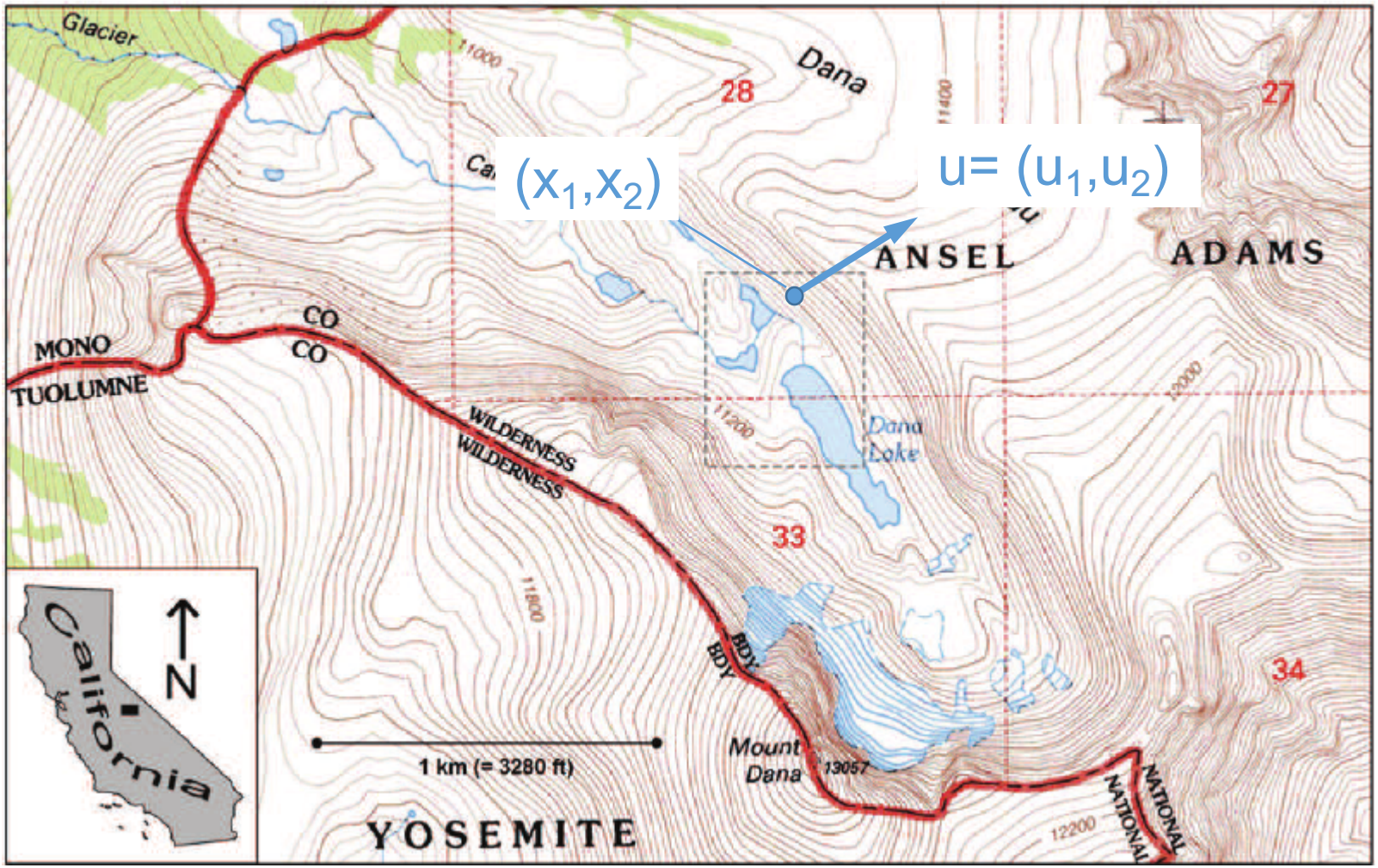
Example

Up or down?



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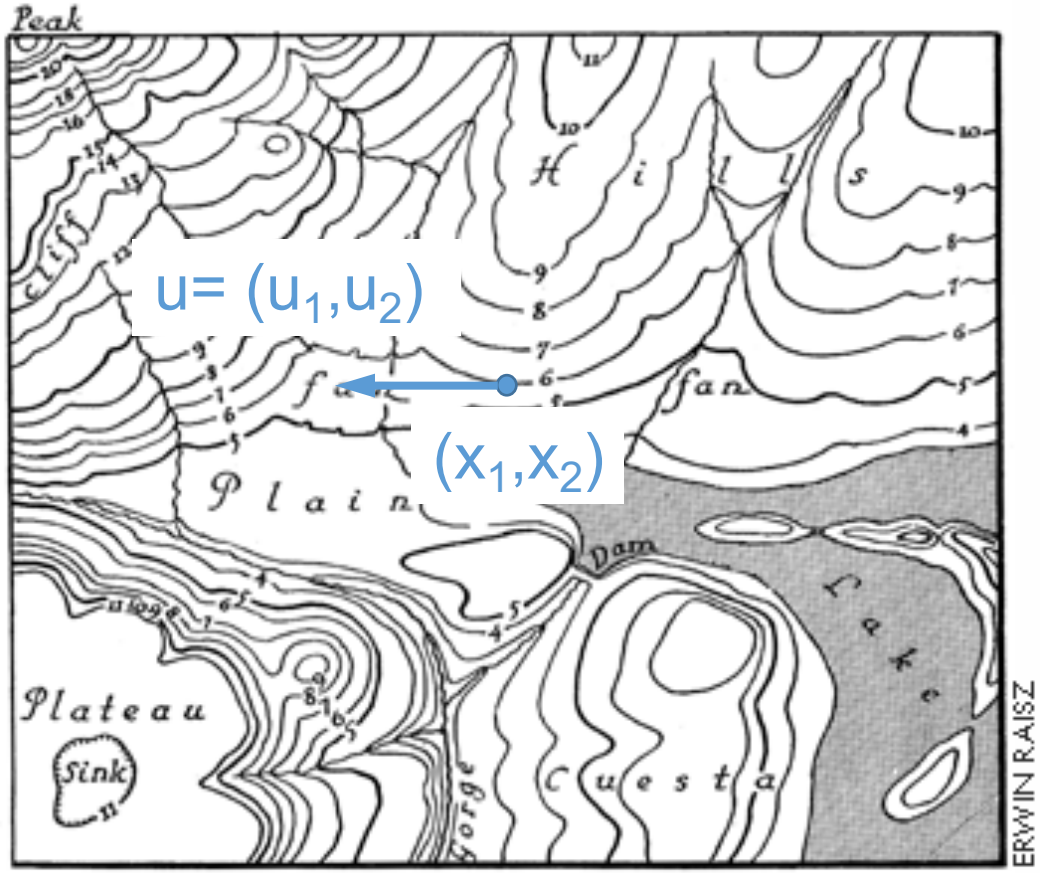
Another …

Up or down?



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Directional Derivatives

- For a differentiable 2D function $f(x_1, x_2)$ the partial derivatives in direction x_i are $\frac{\partial}{\partial x_1} f, \frac{\partial}{\partial x_2} f$
- The derivative in a <u>general direction</u> $u = (u_1, u_2)$ (unit 2D vector) is called the directional derivative $D_u f$ and is defined as:

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

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The Gradient of a function

$$D_u f(x_1, x_2) = \left(\frac{df}{ds}\right)_u = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial s} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial s} =$$

$$= \frac{\partial f}{\partial x_1}u_1 + \frac{\partial f}{\partial x_2}u_2 = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}\right) \cdot (u_1, u_2) = \nabla f(x_1, x_2) \cdot \mathbf{u}$$

This is the dot product of the direction u with a vector that is called the **GRADIENT** and consists of the principle directional derivatives evaluated at (x_1, x_2) :

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

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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 $x = (x_1, x_2)$ we have:

$$D_u f(x) = \nabla f(x) \cdot u$$

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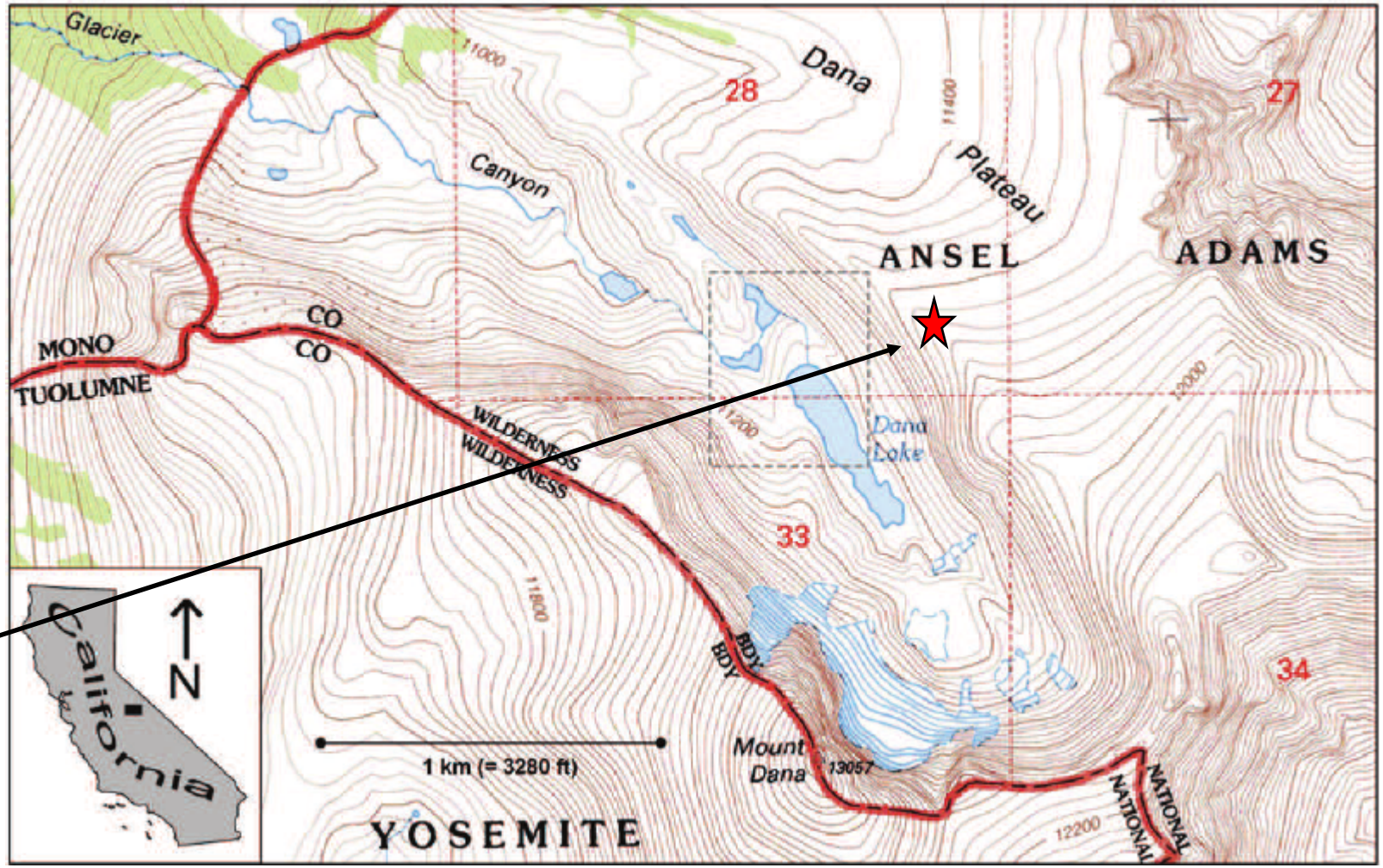
Most Rapid Increase at a point x



The pt x

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Most Rapid Increase at a point x

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

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

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

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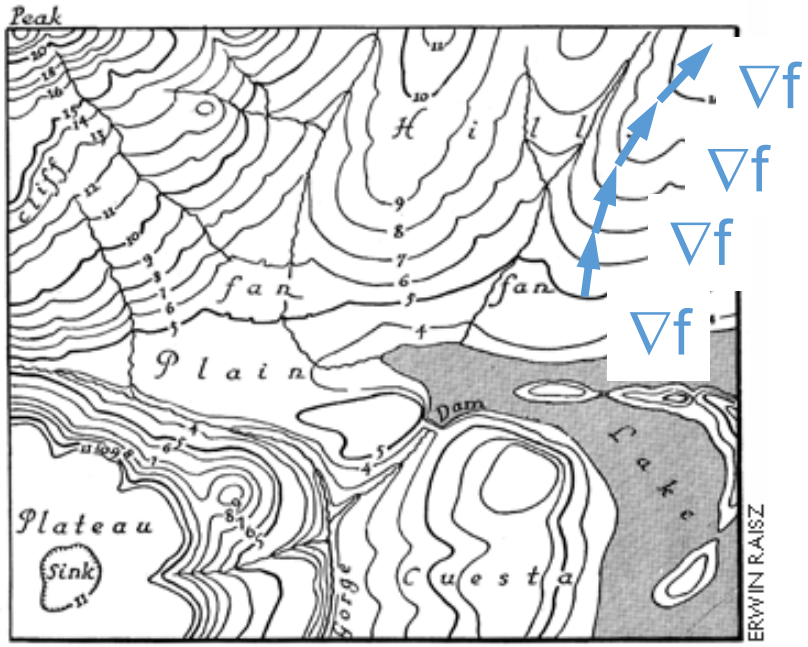
Steepest ascent and Iso-Contours

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



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The gradient of n-dimensional functions

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

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

- 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 the negative of the gradient: $-\nabla f(x_1, x_2 \ \ldots \ x_n)$

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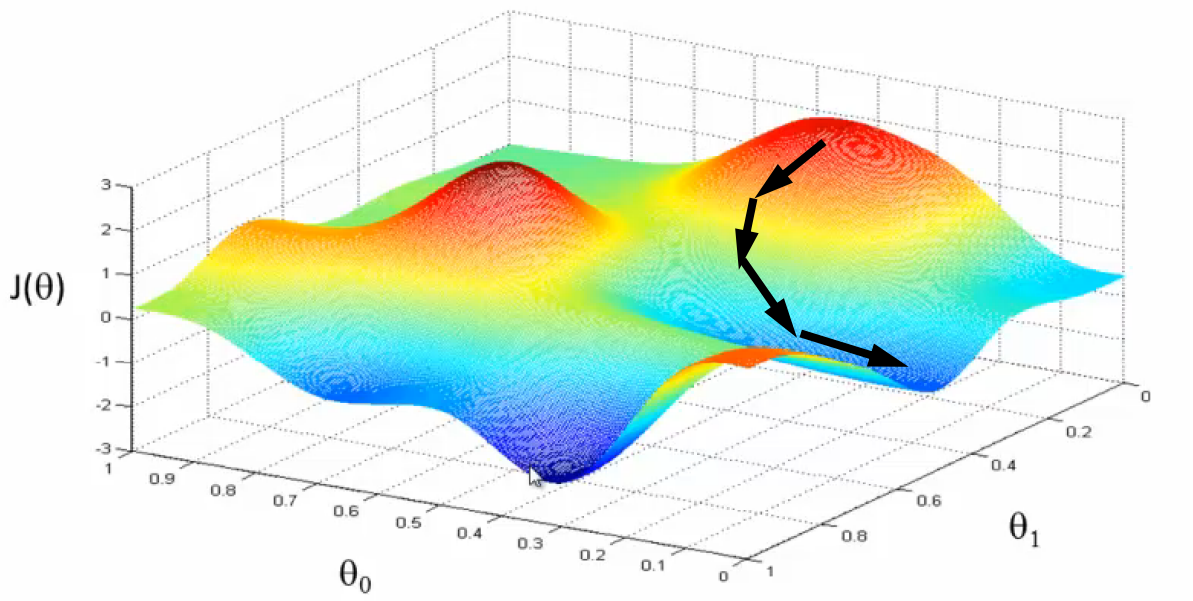
How to find a minimum of a (reasonably smooth) n-dimensional function?

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



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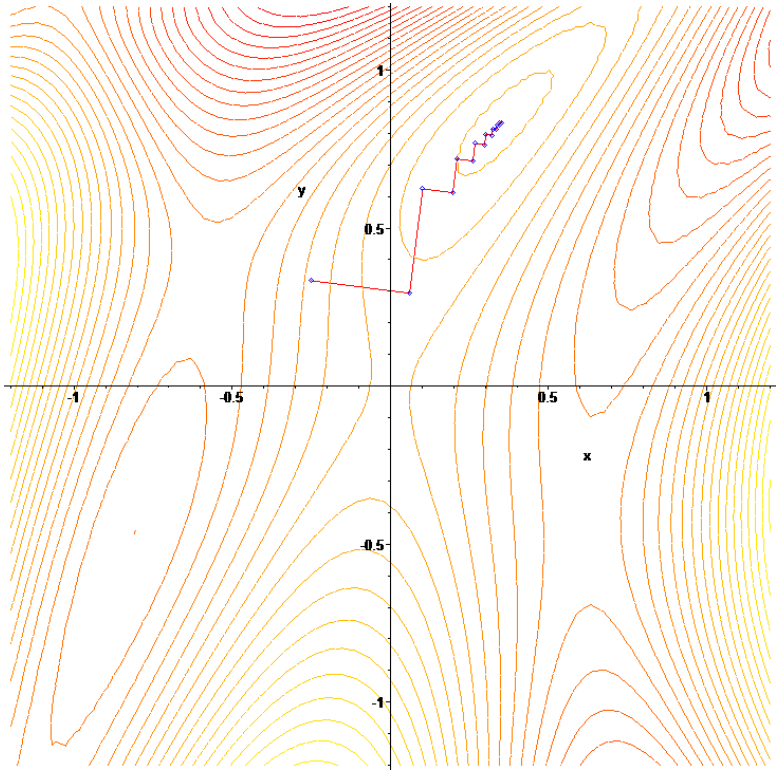
Gradient Descent Steps

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



Back to Minimizing the Cost Function

- Recall that our best hypothesis $\boldsymbol{\theta}^*$ is the one that minimizes the cost function:

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

- This is a real valued function of $\vec{\boldsymbol{\theta}} \in \mathbb{R}^n$
- So - we can start with some initial guess $\overrightarrow{\boldsymbol{\theta}_{\mathbf{0}}^*}$ and then use gradient descent

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Gradient Descent Algorithm

- Start with some value for $\boldsymbol{\theta} = (\theta_0, \theta_1, \theta_2, \ldots, \theta_n)$
- Repeat until you reach a minimum:

  For all j,

  Update $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$

- $\alpha > 0$ 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!

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Minimizing the Cost Function

- Hence, our best hypothesis $\boldsymbol{\theta}^*$ would be the one that minimizes the cost function:

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

- How can we find it?

Calculating the Partial Derivative

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

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

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

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

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Gradient Descent for Linear Regression

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

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

- 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

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Recitation

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

Extra slides/notes

- Correlations
- Pseudo-inverse of a matrix
- Going beyond Linear

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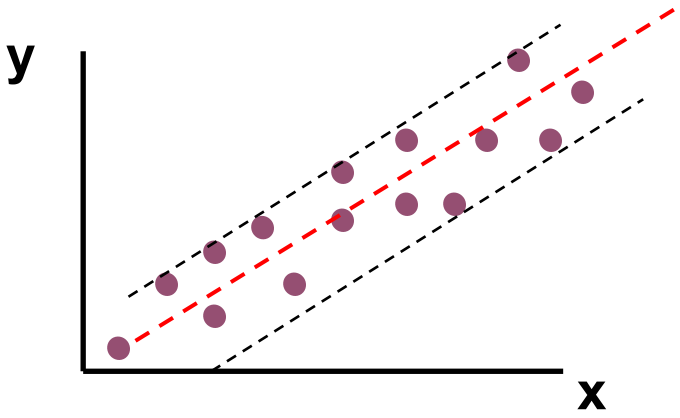
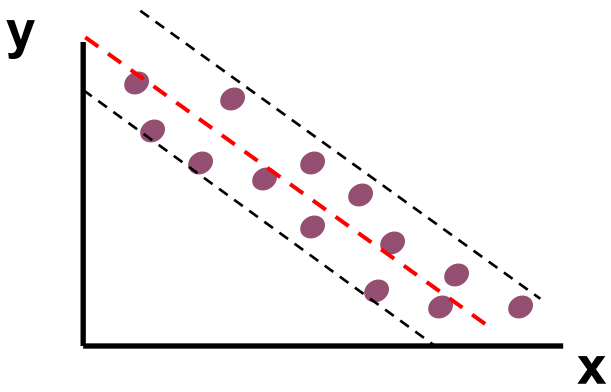
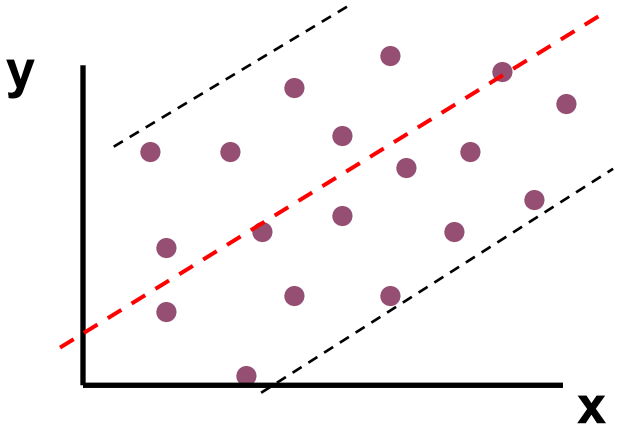
Strong vs. Weak Linear Relationship

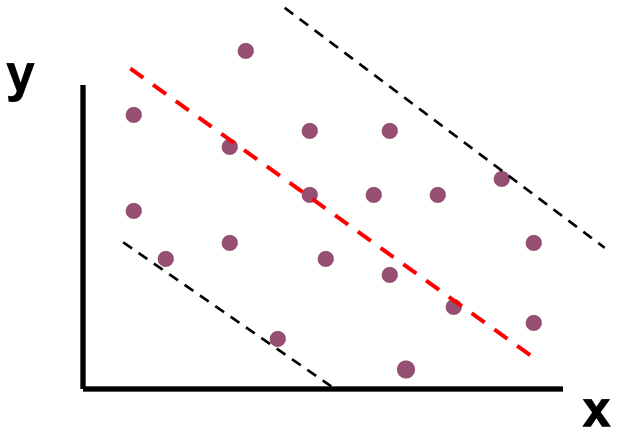
Strong relationships





Weak relationships





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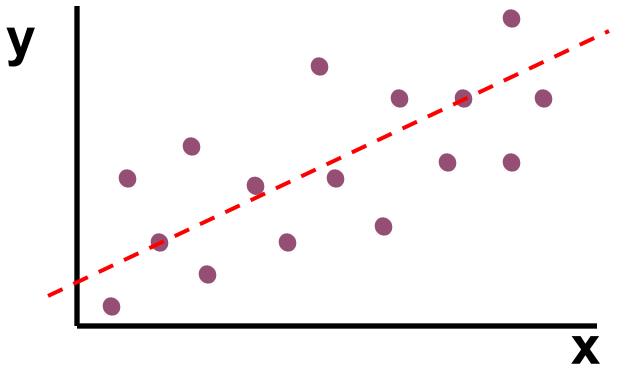
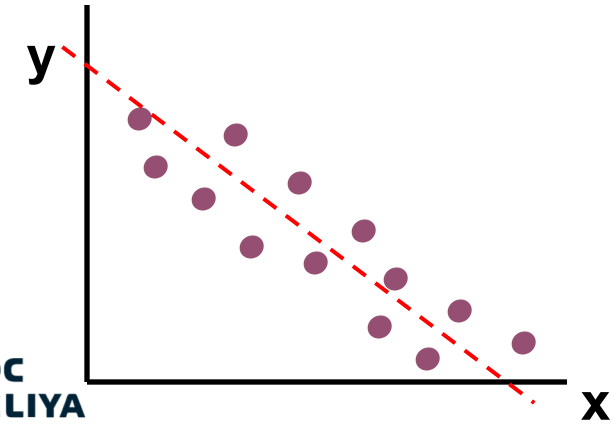
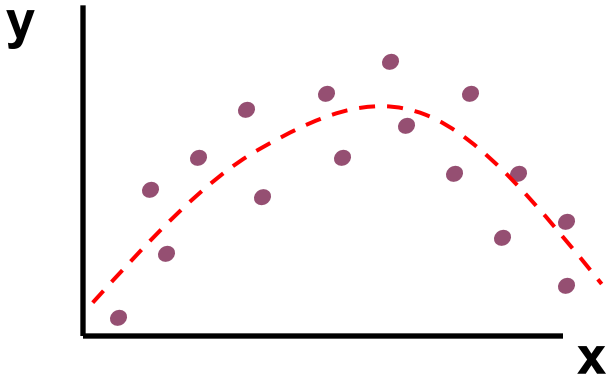
Not Everything is Linear!

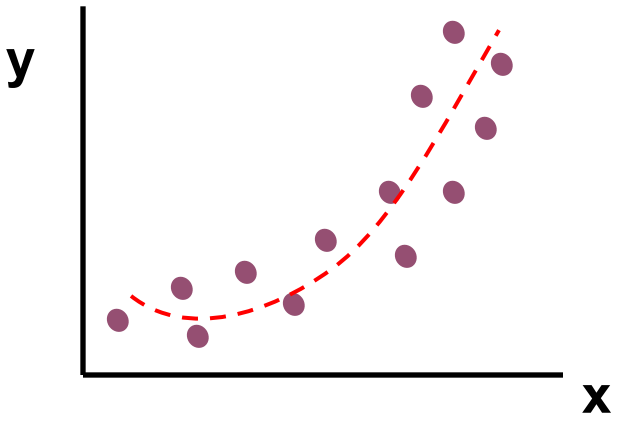
Linear relationships





Curvilinear relationships





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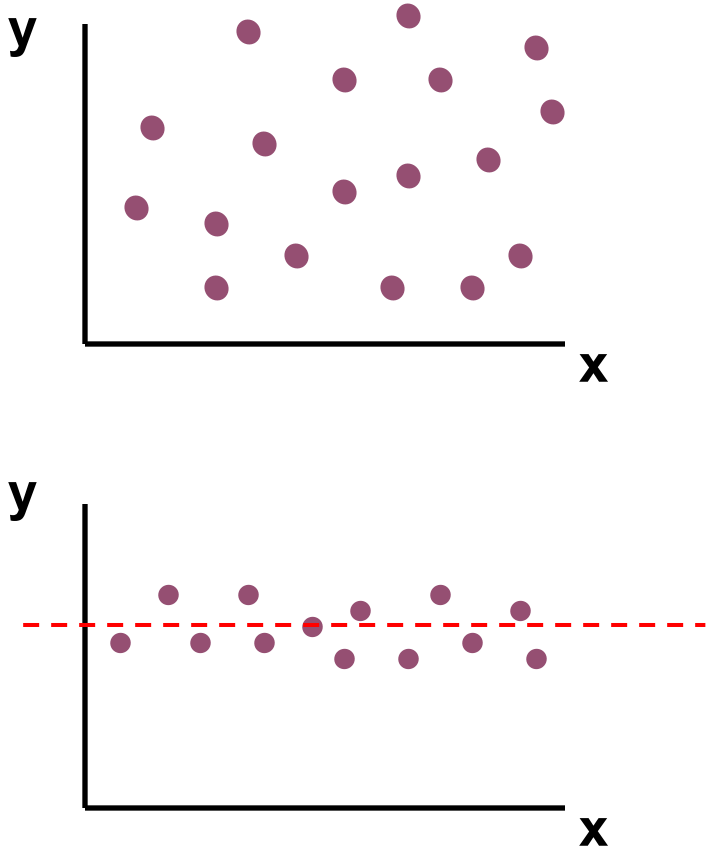
No Evident Relationship



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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

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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

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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

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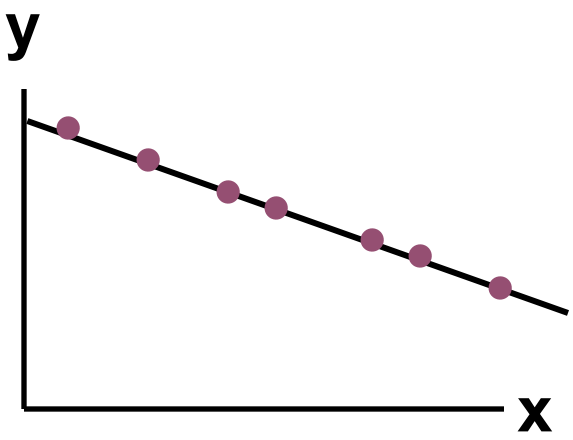
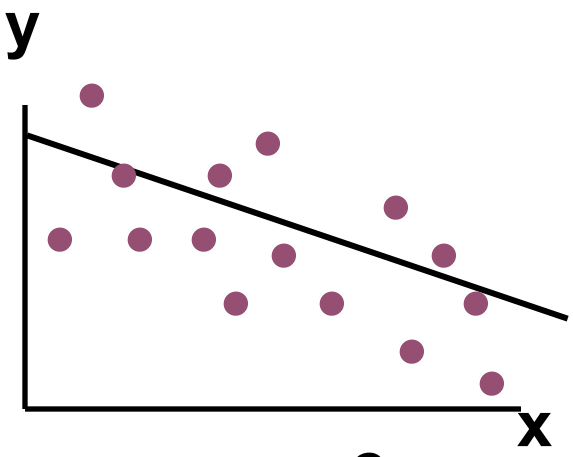
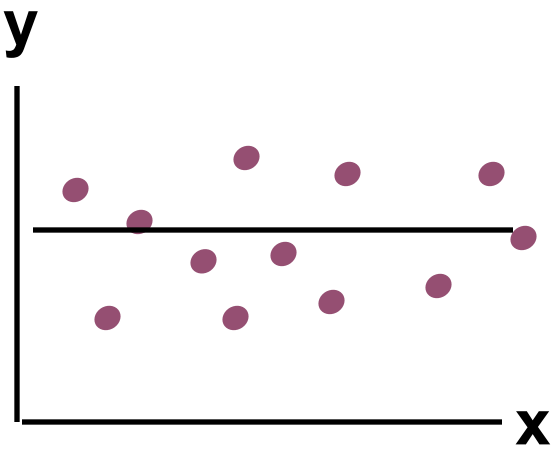
Examples of r Values



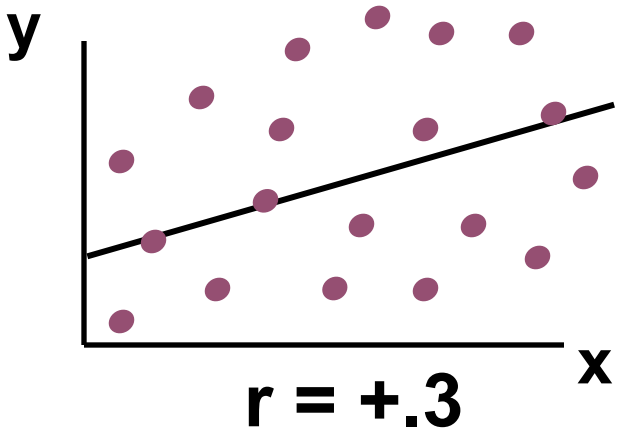
r = -1



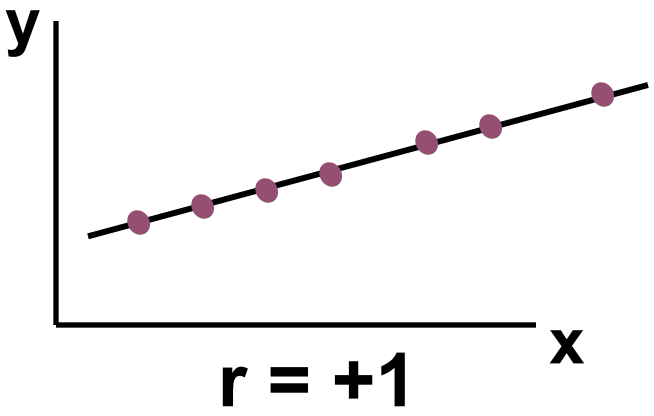
r = -.6



r = 0



r = +.3



r = +1

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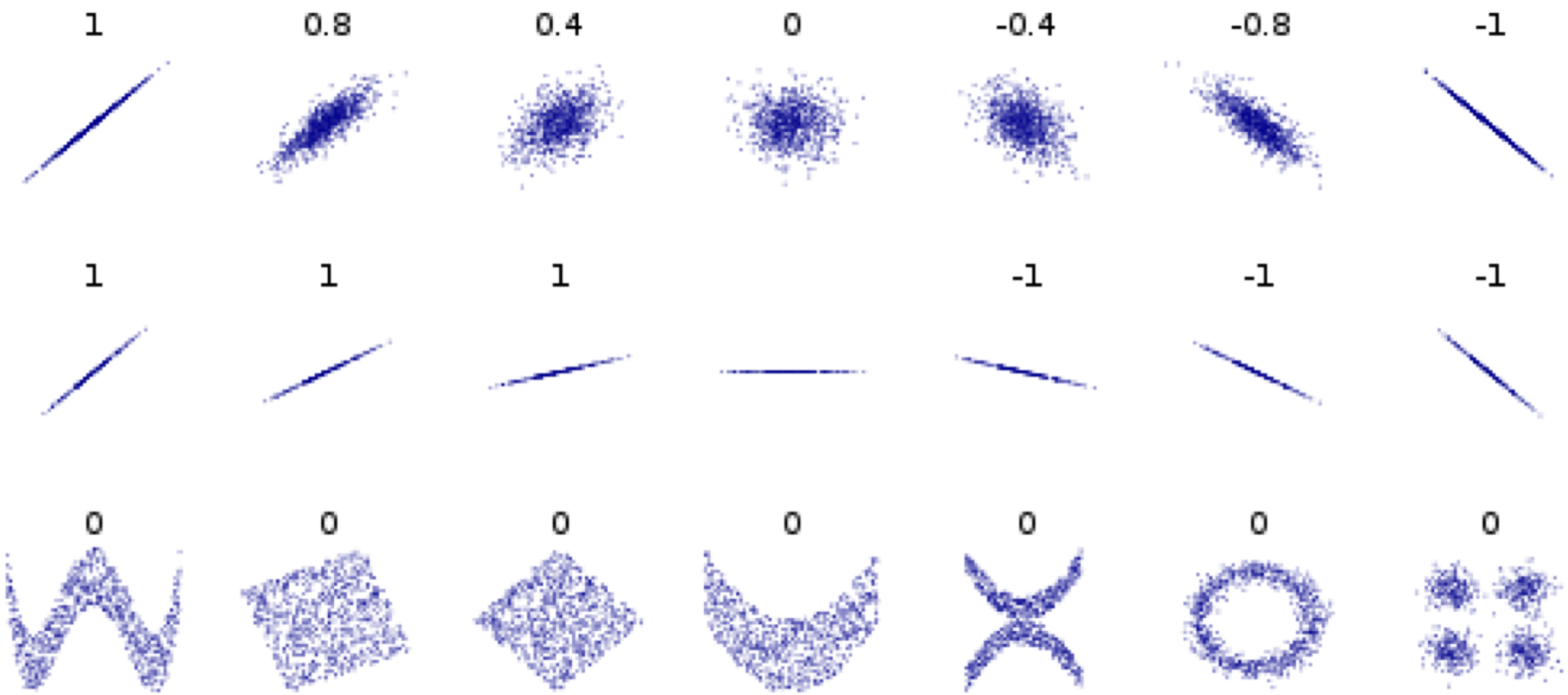
More Complex Relationships May Not Be Captured Using Pearson r



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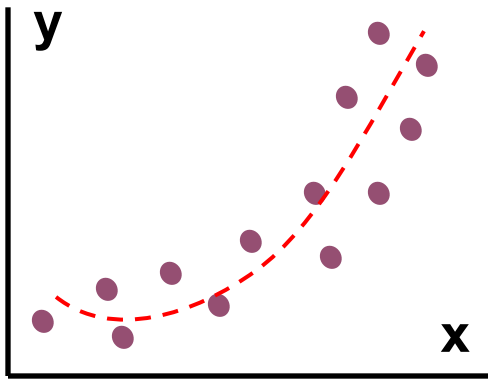
Polynomial Regression

- 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

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



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Other Functions

- We can use other functions of features such as $x^{1/q}$
- We can define functions of sets of variables such as $x_1 x_5 x_7$ or $x_1^2 x_5 x_7^3$
- All of these can be represented as new features and increase the dimension of the entire calculation

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Closed form solution?

$$X \cdot \theta = y$$

$$\begin{pmatrix} x_0^{(1)} & x_1^{(1)} & \dots & x_n^{(1)} \\ x_0^{(2)} & x_1^{(2)} & \dots & x_n^{(2)} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ x_0^{(m)} & x_1^{(m)} & \dots & x_n^{(m)} \end{pmatrix} \begin{pmatrix} \theta_0 \\ \vdots \\ \theta_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \\ \\ y_m \end{pmatrix}$$

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

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Minimum when Derivative is 0

- Lets look at the error vector e = X· $\vec{\boldsymbol{\theta}}$– y
- Minimizing the squared length of this error vector is equivalent to minimizing the sum of squared distance function:

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

- Forming the derivatives yields (see notes):

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

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Pseudo-inverse & the Normal Equation

- Setting the gradient to zero yields the necessary condition for minimum (see notes):

$$\mathbf{X}^T\mathbf{X}\cdot\vec{\boldsymbol{\theta}} = \mathbf{X}^T\overrightarrow{\mathbf{Y}}$$

- Now, X^TX is square and often nonsingular and so we can solve for $\vec{\boldsymbol{\theta}}$ uniquely as:

$$\vec{\boldsymbol{\theta}} = pinv(\mathbf{X})\,\overrightarrow{\mathbf{Y}} \qquad \textbf{where} \qquad pinv(\mathbf{X}) = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T$$

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

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Gradient Descent and Pseudo Inverse

- $\mathbf{X^TX}$ 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.
- Gradinet descent allows parallelization.

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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

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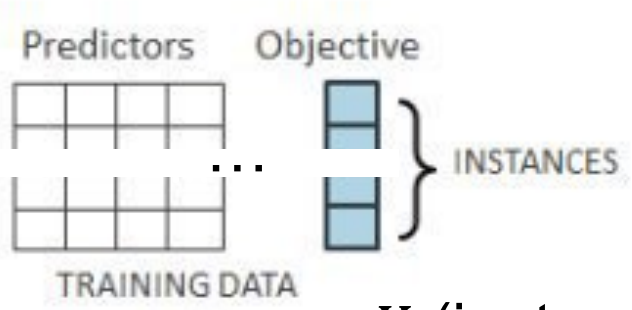
Summary - cont

The execution algorithm:

$y = f(x) = x\theta^T$



X (instances by features)

y (instances)

The learning algorithm (regression)