Machine Learning
V02: Formulating learning problems

Ingredients to learning
Machine learning from scratch

With material from Andrew Y. Ng, Coursera

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InIT Institute of Applied Information Technology (stdm)

Educational objectives

- **Name** the **parts** that make up a machine learning **solution** as well as **concrete instances** of each

- **Understand** the **linear regression** with stochastic **gradient descent** algorithm from scratch

- **Implement** a simple machine **learning algorithm from scratch** (that is, from its mathematical description)

1. INGREDIENTS TO LEARNING

Recap

What is a well-posed learning problem (according to [Mitchell, 1997])?

T:
P:
E:

There are literally thousands of learning algorithms; how can we characterize them?

-
-

Designing a learning solution

High-level view:

Task	Performance measure	training Experience
E.g., • learn playing Tic-Tac-Toe	E.g., • #games won against project team	E.g., • games played against itself

Non-trivial: Use prior knowledge / experience on what works under which conditions.

Non-trivial: What features to use? Then pre-processing takes 80% of the time.

Not so trivial: Often not the standard loss function of your favourite ML library.

Practitioner's view:

Representation: $\mathcal{H}$, features	Evaluation: Loss (objective) function	Optimization: Regime to search $\mathcal{H}$
E.g., • Linear classifier • Sequence of handcrafted board features & end result	E.g., • Squared error between actual and hypothesized outcome	E.g., • Batch gradient descent • Reinforcement learning

Examples for practical components
From [Domingos, 2012]

(Not all possible tuples of $< representation, evaluation, optimization >$ make sense)

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
K-nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search
Hyperplanes	Likelihood	Branch-and-bound
Naive Bayes	Posterior probability	Continuous optimization
Logistic regression	Information gain	Unconstrained
Decision trees	K-L divergence	Gradient descent
Sets of rules	Cost/Utility	Conjugate gradient
Propositional rules	Margin	Quasi-Newton methods
Logic programs		Constrained
Neural networks		Linear programming
Graphical models		Quadratic programming
Bayesian networks		
Conditional random fields		

In a nutshell: Use **experience** (own or read), **experiment** a lot, **constrain** solutions

How to select? (we come back to this question often…)

- Remember V01: No generally best solution available (no free lunch)
  → see V03 and V06 for best practices on model selection
- Guide: *«What **prior knowledge** is **easily** expressed in certain **features** & **models**?»*
- Relieve: **Good & compact features** are more important than model choice

Ask yourself: ***«Do I see** the sought **patterns in** these **features** alone?»*

Formulating a machine learning solution
Quizzy 1/5

Suppose we feed a learning algorithm a lot of historical weather data, and have it **learn to predict weather**. In this setting, **what is** it's training experience ***E***?

- ❑ None of these
- ❑ The probability of it correctly predicting a future date's weather
- ❑ The process of the algorithm examining a large amount of historical weather data
- ❑ The weather prediction task

Formulating a machine learning solution
Quizzy 2/5

Suppose we are working on weather prediction, and use a learning algorithm to **predict tomorrow's temperature** (in degrees Celsius). Would you treat this as a **classification or** a **regression** problem?

- ❑ Classification
- ❑ Regression

Formulating a machine learning solution
Quizzy 3/5

Suppose we are working on stock market prediction, and we would like to **predict whether** or not a particular **stock's price will be higher** tomorrow than it is today. You want to use a learning algorithm for this. Would you treat this as a **classification or a regression** problem?

- ❑ Classification
- ❑ Regression

Formulating a machine learning solution
Quizzy 4/5

Some of the problems below are best addressed using a supervised learning algorithm, and the others with an unsupervised algorithm. **Which** of the following **would you apply supervised learning** to?

- ❑ Examine a web page, and classify whether the content on the web page should be considered “child friendly” (e.g., non-pornographic etc.) or ”adult”
- ❑ Examine a large collection of emails that are known to be spam email, to discover if there are sub-types of spam mail
- ❑ In farming, given data on crop yields over the last 50 years, learn to predict next year’s crop yields
- ❑ Take a collection of 1’000 essays written on the Swiss economy, and find a way to automatically group these essay into a small number of groups that are somehow “similar” or “related”

Formulating a machine learning solution
Quizzy 5/5

Many substances that can burn…

…(such as gasoline and alcohol) have a chemical structure based on carbon atoms. For this reason they are called hydrocarbons. A chemist wants to **understand how the number of carbon atoms in a molecule affects how much energy is released** when that molecule combusts (meaning that it is burned). The chemist obtained the dataset below. In the column on the right, "kJ/mol" is the unit measuring the amount of energy released.

- ❑ Is it classification or regression?
- ❑ What is X, Y (the training data)?

- ❑ What could be the relationship? How to gain first insight?

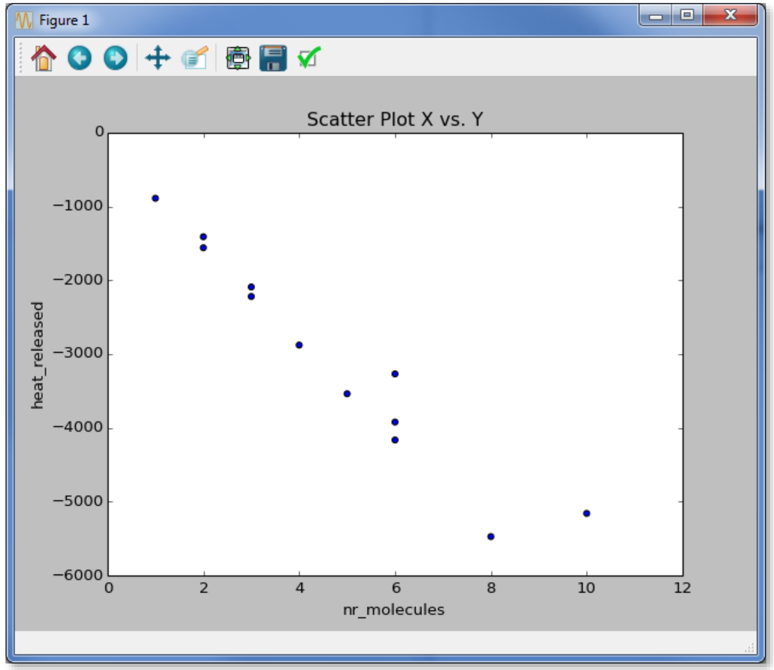
Name of molecule	Number of carbon atoms in molecule	Heat released when burned (kJ/mol)
Methane	1	-890
Ethene	2	-1411
Ethane	2	-1560
Propane	3	-2220
Cyclopropane	3	-2091
Butane	4	-2878
Pentane	5	-3537
Benzene	6	-3268
Cycloexane	6	-3920
Hexane	6	-4163
Octane	8	-5471
Napthalene	10	-5157

Getting first insights
Example: Quizzy 5/5

```
import matplotlib.pyplot as plt
import pandas as pd

data_frame = pd.read_excel("hydrocarbons.xlsx")

plt.scatter(data_frame['nr_molecules'],
data_frame['heat_release'])
plt.title("Scatter Plot X vs. Y")
plt.xlabel(data_frame.columns[1])
plt.ylabel(data_frame.columns[2])
plt.show()
```



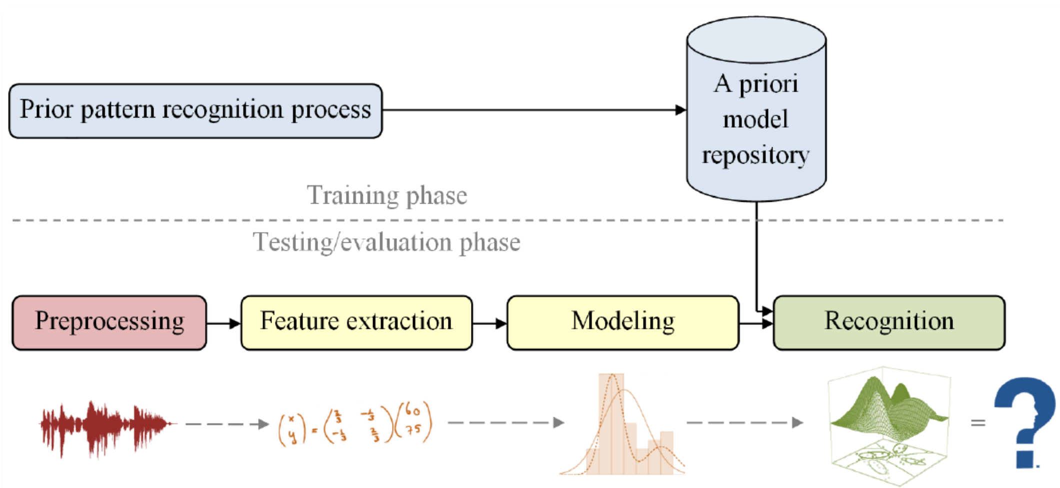
Low-hanging fruits

- Exploratory data analysis (visualization) → this and next slide
- Trying simpler models first → next section

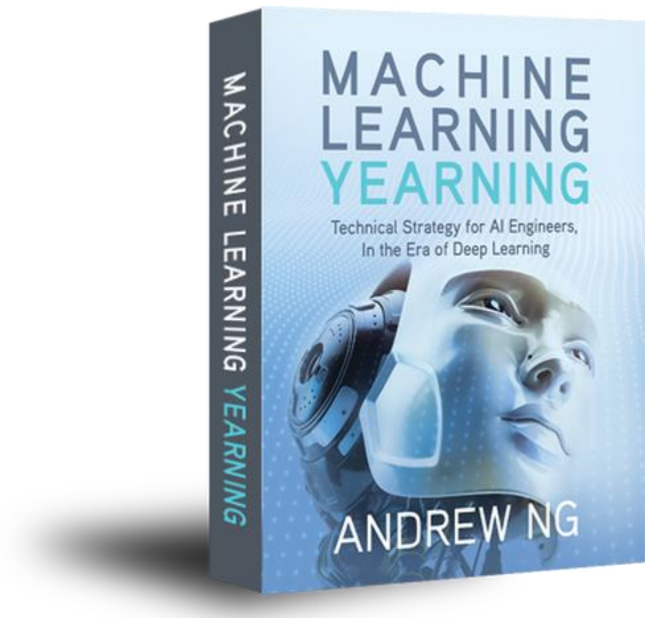
The Machine Learning development process
Exploration & experimentation

Necessity of a distinct conceptual approach
- Modeling data ≠ {software dev., business process mngmt., data base design, stat. analysis, …}

In a nutshell
- Focus on **systematic experimentation** and **rigorous evaluation** → automatized
- Best implemented by (a **pipeline of**) **scripts** → UNIX command line approach
- Data **exploration** and **rapid prototyping** is key → IPython (see appendix of V03)



2. MACHINE LEARNING FROM SCRATCH



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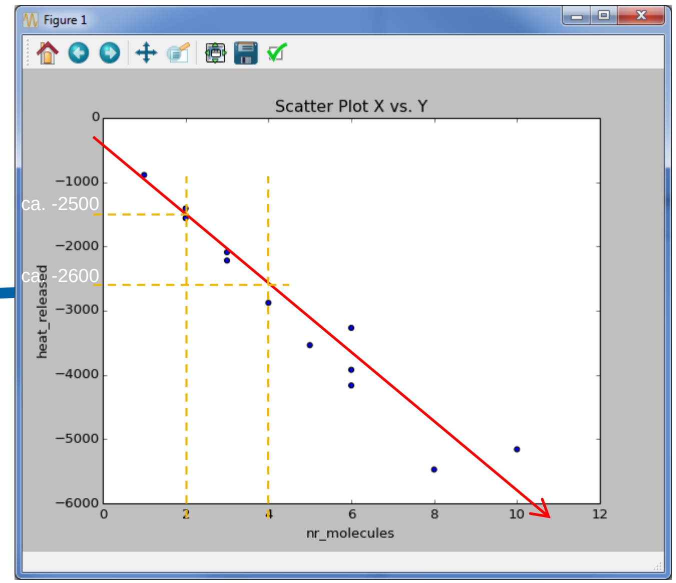
Carbon and combustion
Continuous example for this section

We need a solid understanding of $< Representation, Evaluation, Optimization >$

Thus, this section explores
- …a «**straight line fit**» as a simplistic model
- …all the details of **how to train** it
- …to get a feeling of **ML apart from libraries**



Observations
- The data shows a linear trend
- The gradient is roughly $\frac{-2500+2600}{2-4} = -50$

Conclusions
- Labeled data available → supervised learning
- Contiuous valued output → regression

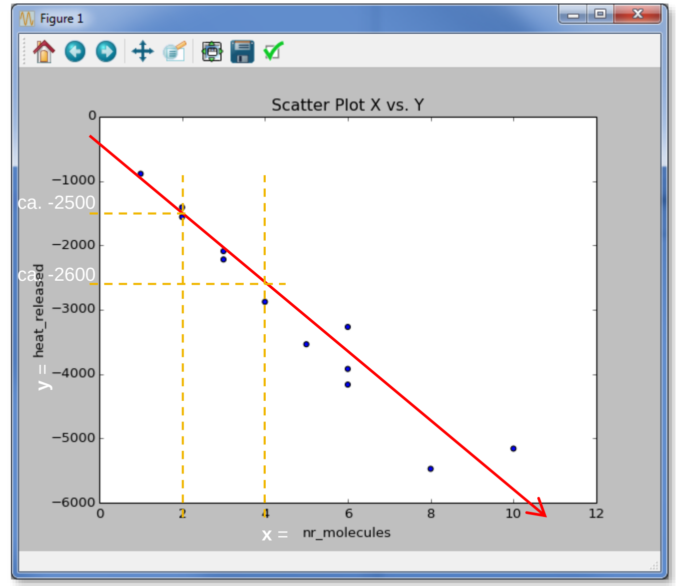
➔ Linear regression could be a first try

How to represent h?

..in the case of univariate linear regression

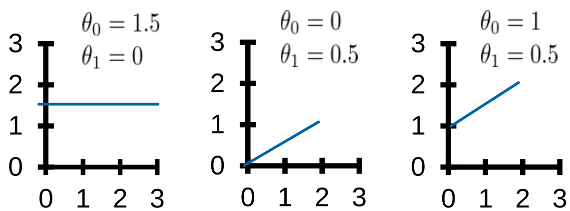
$$h(x, \vec{\theta}) = \theta_0 + \theta_1 x$$

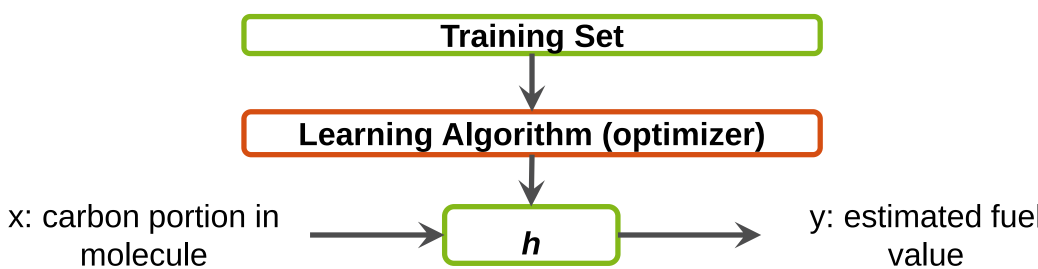
- θ_0 = intercept, θ_1 = gradient



How to choose parameters θ_0, θ_1?

- Parameters correspond with different fits





Aliases: loss function, objective function $*(-1)$

Cost function J

Driver of the optimization

Idea

- **Choose $\boldsymbol{\theta_0}$, $\boldsymbol{\theta_1}$ so** that $\boldsymbol{h(x)}$ **is close to $\boldsymbol{y}$** for the training examples (x, y)
- Let a function $\boldsymbol{J(parameters)}$ **number the cost of errors** made for specific parameters

We didn't mention a few parameters here → see below for complete list

$h(x, \vec{\theta}) = \theta_0 + \theta_1 x$

squared error

$$J(\theta_0, \theta_1) = \frac{1}{2N} \sum_{i=1}^{N} \left(h\left(x_i, \vec{\theta}\right) - y_i\right)^2$$

/2 for mathematical beauty (ease)…

average over all N examples

Precise objective

- **Minimize $\boldsymbol{J}$** w.r.t. θ_0, θ_1
- In terms of V01:
  - $L(\hat{y}, y) = (\hat{y} - y)^2$ is the squared error loss function
  - $J(\theta_0, \theta_1, h, X, Y, L) = E_{emp}\left(h(\vec{\theta}), X, Y, L\right) = \frac{1}{N}\sum_{i=1}^{N} L\left(h\left(x_i, \vec{\theta}\right), y_i,\right)$ is the **cost of error** with **explicit** respect to **all parameters**: Measured in terms of the empirical error over the training set (X, Y) according to the squared error loss function L for a particular hypothesis h

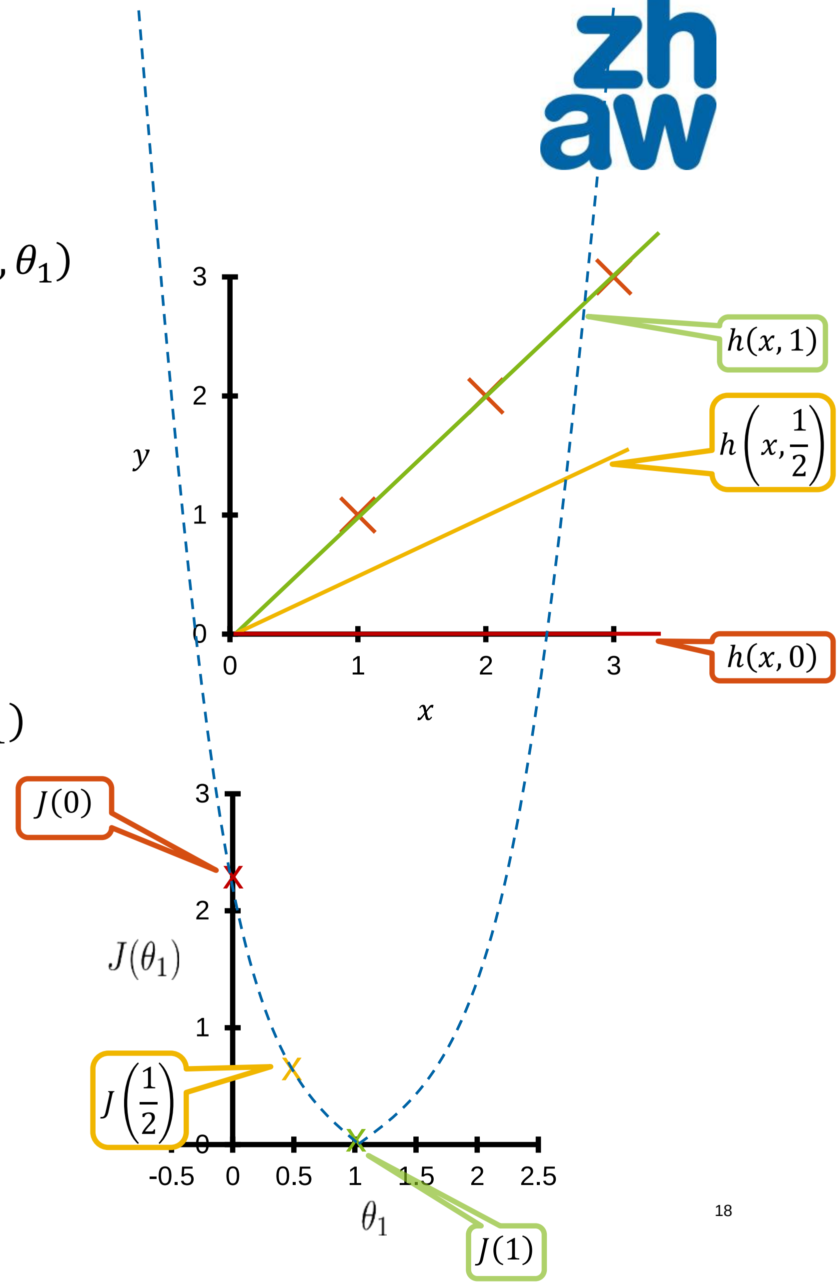
Simplified version to gain intuition
Fixed intercept at (0,0)

- Hypothesis: $h(x, \theta_1) = 0 + \theta_1 x$
- Parameter: θ_1
- Cost: $J(\theta_1) = \frac{1}{2N} \sum_{i=1}^{N} (h(x_i, \theta_1) - y_i)^2$
- Goal: $\underset{\theta_1}{\text{minimize}}\, J(\theta_1)$

Example values of J

- $J(1) = \frac{1}{6} \sum_{i=1}^{3} (h(x_i, 1) - y_i)^2$
  $= \frac{1}{6} \sum_{i=1}^{3} (x_i - y_i)^2$
  $= \frac{1}{6} \left((1-1)^2 + (2-2)^2 + (3-3)^2\right) = 0$
- $J\left(\frac{1}{2}\right) = \cdots = \frac{1}{6}\left(\left(\frac{1}{2} - 1\right)^2 + (1-2)^2 + \left(\frac{3}{2} - 3\right)^2\right)$
  $= \frac{1}{6} \cdot \frac{7}{2} \approx 0.58$
- $J(0) = \cdots = \frac{1}{6}(1^2 + 2^2 + 3^2) = \frac{1}{6} \cdot 14 \approx 2.33$
- …

- $h(x, \theta_1)$
- $J(\theta_1)$

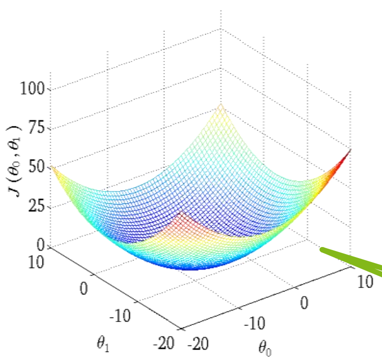


Back to two parameters

- Hypothesis: $h(x,\vec{\theta}) = \theta_0 + \theta_1 x$
  ➔ For fixed $\vec{\theta}$, this is a **function of x**

- Parameters: θ_0, θ_1

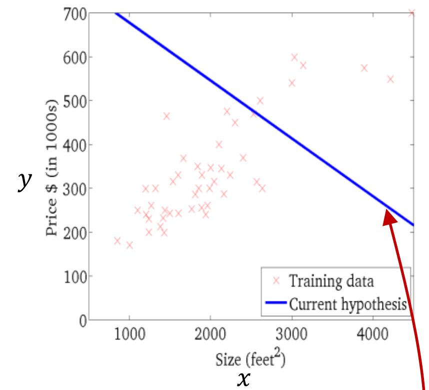
- Cost: $J(\theta_0,\theta_1) = \frac{1}{2N}\sum_{i=1}^{N}\left(h(x_i,\vec{\theta}) - y_i\right)^2$
  ➔ For fixed x, this is a **function of $\vec{\theta}$**



- Goal: $\underset{\theta_0,\theta_1}{\text{minimize}}\, J(\theta_0,\theta_1)$

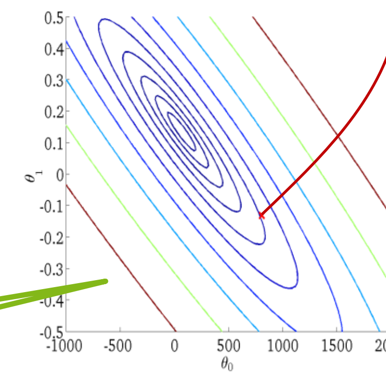
Example: Housing prices (y) per size (x)

- $h(x,\vec{\theta})$



$h(x, 800, -1.5)$

- $J(\theta_0,\theta_1)$



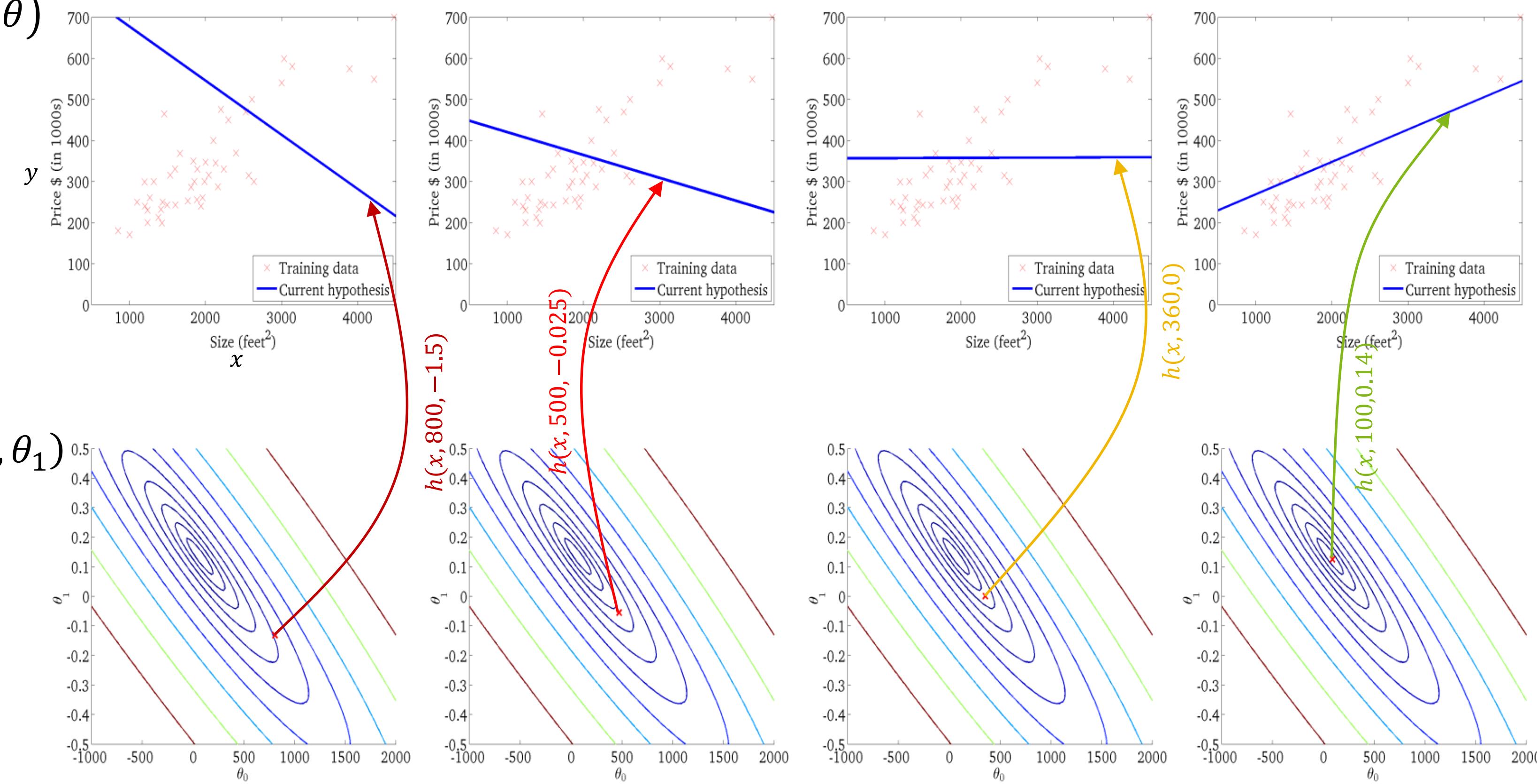
J is a convex (bowl-shaped) function of 2 variables → 3D

…and its 2D visualization as a contour plot

Back to two parameters
contd.

Example: Housing prices (y) per size (x)

- $h(x, \vec{\theta})$
- $J(\theta_0, \theta_1)$



Optimization by gradient descent

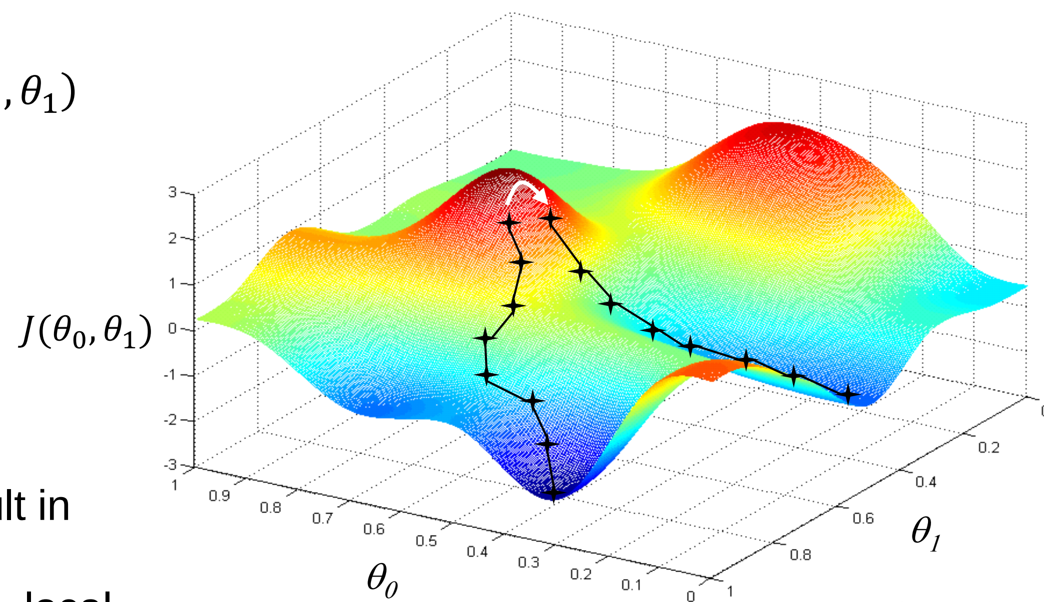
Numerical optimization

Have: Some function $J(\theta_0, \theta_1)$

Want: $\underset{\theta_0, \theta_1}{\text{minimize}}\, J(\theta_0, \theta_1)$

Algorithm

- Start with some θ_0, θ_1 (e.g., $(0{,}0)$)
- Keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$
  → Direction: steepest descent
- End: Hopefully at a minimum



Observations

- Small changes in starting point result in different **local minima**
- Assumption: cost surface is smooth, local minima are ok

Gradient descent algorithm

Pseudo code for gradient descent

- ```
  repeat until convergence:
      for j:=0..1:
          θ̂_j := θ_j − α · ∂/∂θ_j J(θ_o, θ_1)
      for j:=0..1:
          θ_j := θ̂_j
  ```
- $\frac{\partial}{\partial \theta_j} J(\theta_o, \theta_1)$ is the partial derivative of J w.r.t. θ_j
- $\alpha > 0$ is called the learning rate (it is a data-dependent hyper parameter of the algorithm)
- Important: **simultaneous update**!

```
tmp_0 := θ_0 − α · ∂/∂θ_0 J(θ_o, θ_1)
tmp_1 := θ_1 − α · ∂/∂θ_1 J(θ_o, θ_1)
θ_0 := tmp_0
θ_1 := tmp_1
```

```
θ_0 := θ_0 − α · ∂/∂θ_0 J(θ_o, θ_1)
θ_1 := θ_1 − α · ∂/∂θ_1 J(θ_o, θ_1)
```

Problem: changed $\boldsymbol{\theta_0}$ is already used to estimate new $\boldsymbol{\theta_1}$

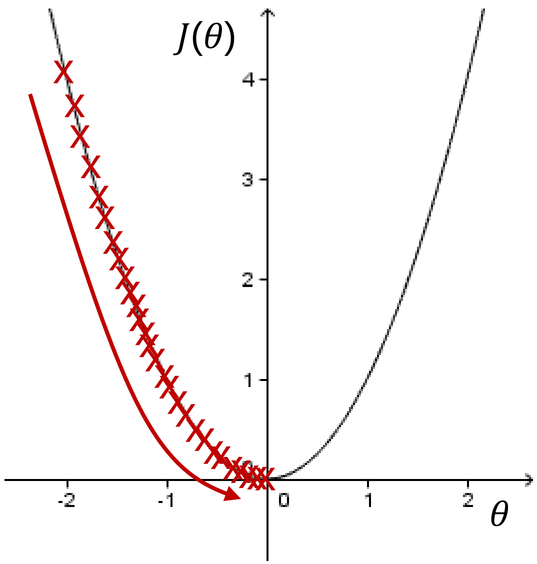
Why not solving it analytical?

- Numerical optimization **scales better** to larger data sets
- Gradient descent also works for h's without analytical solution (e.g., neural networks)
```

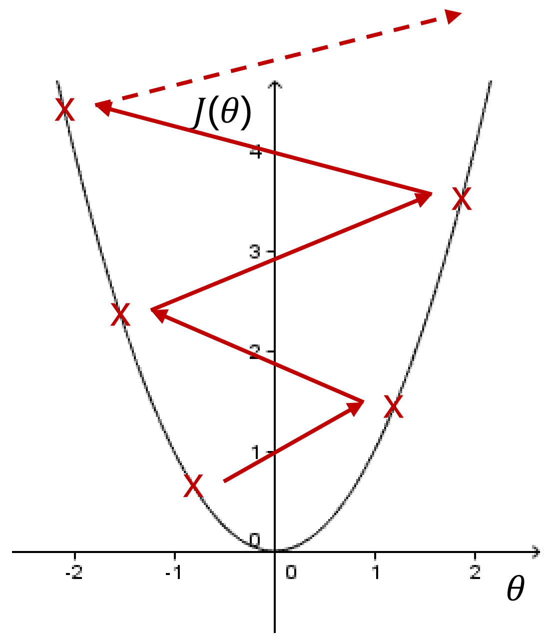
Intuition behind gradient descent formulae (II)

Effect of the learning rate α

- α too **small**
  ➔ gradient descent is **slow**



- α too **large**
  ➔ gradient descent **overshoots** minimum
  ➔ no convergence or divergence!



Gradient descent for univariate linear regression
Formal overview

Ingredients

- Representation
  - $h(x, \vec{\theta}) = \theta_0 + \theta_1 x$
- Evaluation
  - $J(\theta_0, \theta_1) = \frac{1}{2N}\sum_{i=1}^{N}\left(h\left(x_i, \vec{\theta}\right) - y_i\right)^2$
  - $\frac{\partial}{\partial\theta_0}J(\theta_0, \theta_1) = \frac{1}{N}\sum_{i=1}^{N}\left(h\left(x_i, \vec{\theta}\right) - y_i\right)\cdot 1$
  - $\frac{\partial}{\partial\theta_1}J(\theta_0, \theta_1) = \frac{1}{N}\sum_{i=1}^{N}\left(h\left(x_i, \vec{\theta}\right) - y_i\right)\cdot x_i$
- Optimization
  -

```
repeat until convergence:
    for j:=0..1:
        θ̂_j := θ_j − α · ∂/∂θ_j J(θ_o, θ_1)
    for j:=0..1:
        θ_j := θ̂_j
```

$$\frac{\partial}{\partial\theta_j}J(\theta_o, \theta_1) = \frac{\partial}{\partial\theta_j}\frac{1}{2N}\sum_{i=1}^{N}\left(h(x_i, \vec{\theta}) - y_i\right)^2$$

→ see appendix

$\frac{\partial}{\partial\theta_0}h(x_i, \vec{\theta})$

$\frac{\partial}{\partial\theta_1}h(x_i, \vec{\theta})$

```
repeat until convergence:
    θ̂_0 := θ_0 − α · 1/N Σ_{i=1}^N (h(x_i, θ) − y_i)
    θ̂_1 := θ_1 − α · 1/N Σ_{i=1}^N (h(x_i, θ) − y_i) · x_i
    θ_0 := θ̂_0
    θ_1 := θ̂_1
```

Batch gradient descent: uses all training examples at once (as opposed to stochastic gradient descent, which uses small chunks called "mini-batches"…)

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Review

- A **learning solution** needs a **representation**, an **evaluation** function and an **optimizer**

- These can be derived from the formulation of a **well-posed learning problem** as **task**, **performance** measure and training **experience**

- There is **no general solution** to deriving these concrete methods. It is problem (data-) dependent and relies on prior knowledge
- **Valid guides** are the **characteristics of methods** (inductive bias, VC theory), **experience** / **best practices** and **prior knowledge**

- **Gradient descent** is a general-purpose optimizer; implementation details (**simultaneous updates**) and **hyper parameters** are practically very relevant

P02.1: Implementing ML from scratch

Work through exercise P02.1:

- Implement the algorithms derived in this chapter just using the given formal descriptions (i.e., slide 23)
- Reflect on the methods: How transferable are experiences from one data set to the next?
- Reflect on your implementation: What took you the most time? Which part was easy for you?

APPENDIX

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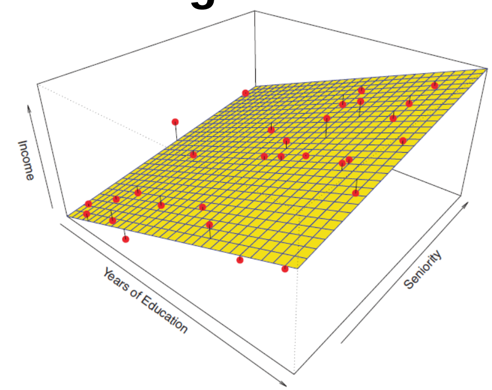
Remark: Different levels of inductive bias

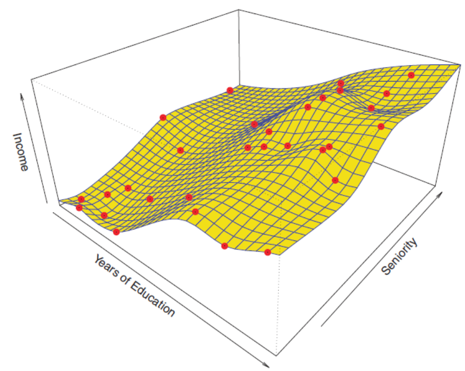
Are there more general forms of prior knowledge that universally guide learning?

application level

fundamental level

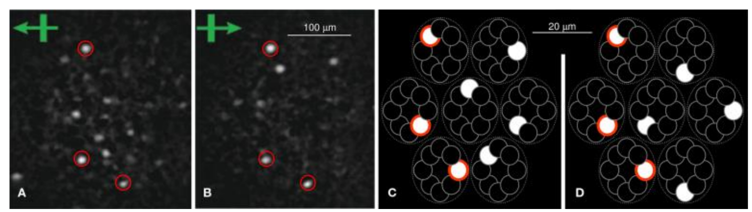
there's a linear relationship between inputs & outputs





the hypothesis space is **smooth**

learn **sparse**, **distributed** representations



Intuition behind gradient descent formulae (I)

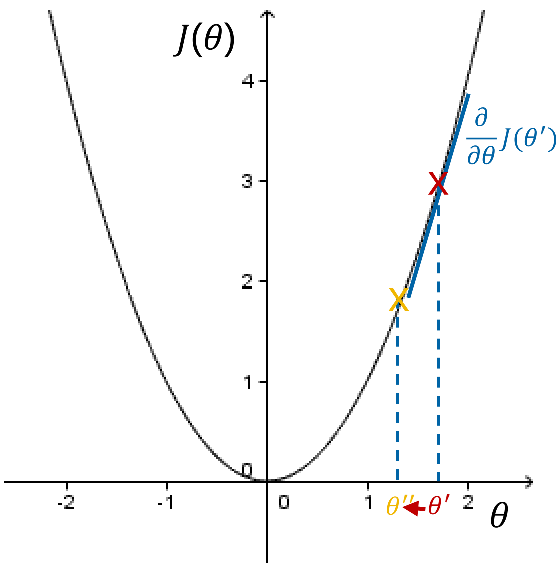
Signs and α automatically care for proper *descent*

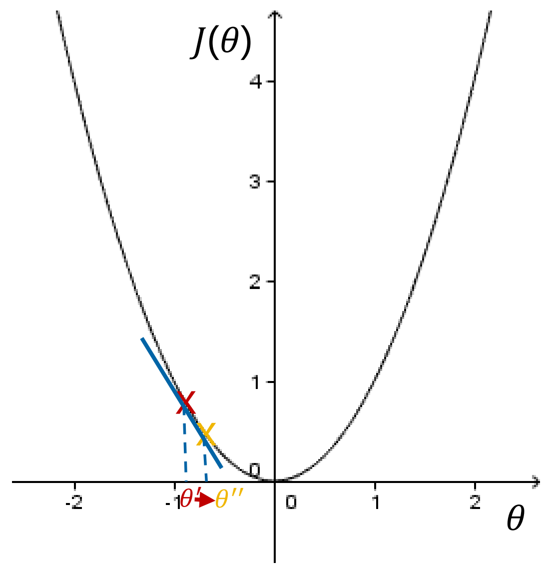
next value   current value

- $\theta'' := \theta' - \underbrace{\alpha}_{} \cdot \underbrace{\frac{\partial}{\partial \theta'} J(\theta')}_{}$

positive numbers

- $\theta'' := \theta' - \alpha \cdot \underbrace{\frac{\partial}{\partial \theta'} J(\theta')}_{\text{negative slope}}$





- As we approach the minimum, steps automatically get smaller ➔ α may be fixed over time

Derivative of J w.r.t. θ_j

$$\frac{\partial}{\partial\theta_j}J(\theta_o,\theta_1)=\frac{\partial}{\partial\theta_{\boldsymbol{j}}}\frac{1}{2N}\sum_{i=1}^{N}\left(h\left(x_i,\vec{\theta}\right)-y_i\right)^2=\sum_{i=1}^{N}\frac{\partial}{\partial\theta_{\boldsymbol{j}}}\frac{1}{2N}\left(h\left(x_i,\vec{\theta}\right)-y_i\right)^2$$

Chain rule: $f\left(g(x)\right)'=f'\left(g(x)\right)\cdot g'(x)$

$$=\sum_{i=1}^{N}\frac{2}{2N}\left(h\left(x_i,\vec{\theta}\right)-y_i\right)\cdot\frac{\partial}{\partial\theta_{\boldsymbol{j}}}\left(h\left(x_i,\vec{\theta}\right)-y_i\right)$$

$$=\sum_{i=1}^{N}\frac{1}{N}\left(h\left(x_i,\vec{\theta}\right)-y_i\right)\cdot\frac{\partial}{\partial\theta_{\boldsymbol{j}}}h\left(x_i,\vec{\theta}\right)$$

$$=\begin{cases} j=0 \quad\longrightarrow\quad \dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\left(h\left(x_i,\vec{\theta}\right)-y_i\right)\cdot 1 \\ j=1 \quad\longrightarrow\quad \dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\left(h\left(x_i,\vec{\theta}\right)-y_i\right)\cdot x_i \end{cases}$$

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Choosing cost functions

Ideal properties of a cost function

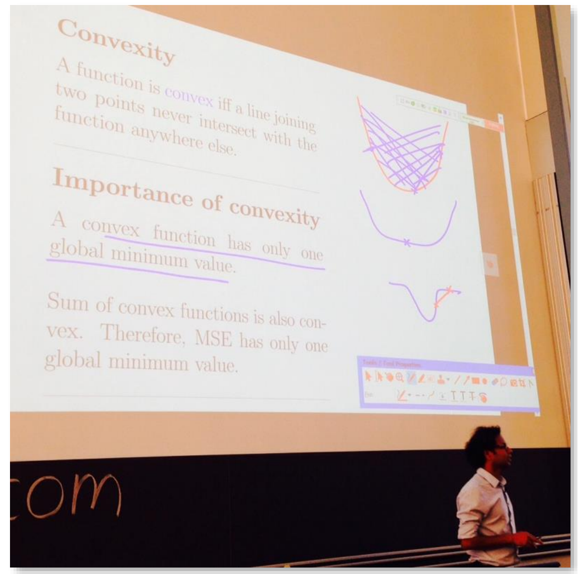
1. Being **easy to optimize** → should be a *convex* function
2. Assigning **equal cost to far and very far** off examples → makes it **robust to outliers**

Cost functions in practice

- MSE (mean-squared error) is almost always used for regression
  → it only exhibits property 1
- Making MSE level off would make the function non-convex
  → when using **MSE**, one has to care for **outliers** during **pre-processing**

➔ Cost function design is important
(because the usual one might not capture the problem well)

➔ …but care has to be taken to make it mathematically sound!



Emti Khan, EPFL, at his introductory ML course during Zurich ML Meetup #18, 25.08.2015

Further reading

- Boyd & Vandenberghe, *«Convex Optimization»*, 2004 → ch. 3
- Bertsekas, *«Convex Optimization Algorithms»*, 2015 → ch. 1
- Chu, *«Machine Learning Done Wrong»*, 2015

Examples of built-to-purpose cost functions
from [Mitchell, 1997], chapter 6.5

Certain well-known cost functions can be justified theoretically using Bayesian reasoning by showing optimality under certain assumptions:

Minimizing *squared error*
- Yields maximum likelihood (ML) hypothesis assuming Gaussian noise on the labels
  Example: Training *linear regression* to fit a straight line

Minimizing *cross entropy*
- Yields ML hypothesis assuming the labels are a probabilistic function of the training examples
- Example: Training a *neural network* to predict probabilities

CMU's Tom Mitchell, author of one of the most instructive machine learning books.

→ see appendix of V03