UNIVERSITAT DE BARCELONA

# Course. Introduction to Machine Learning
# Lecture 6. A gentle introduction to Supervised Learning

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# Acknowledgements

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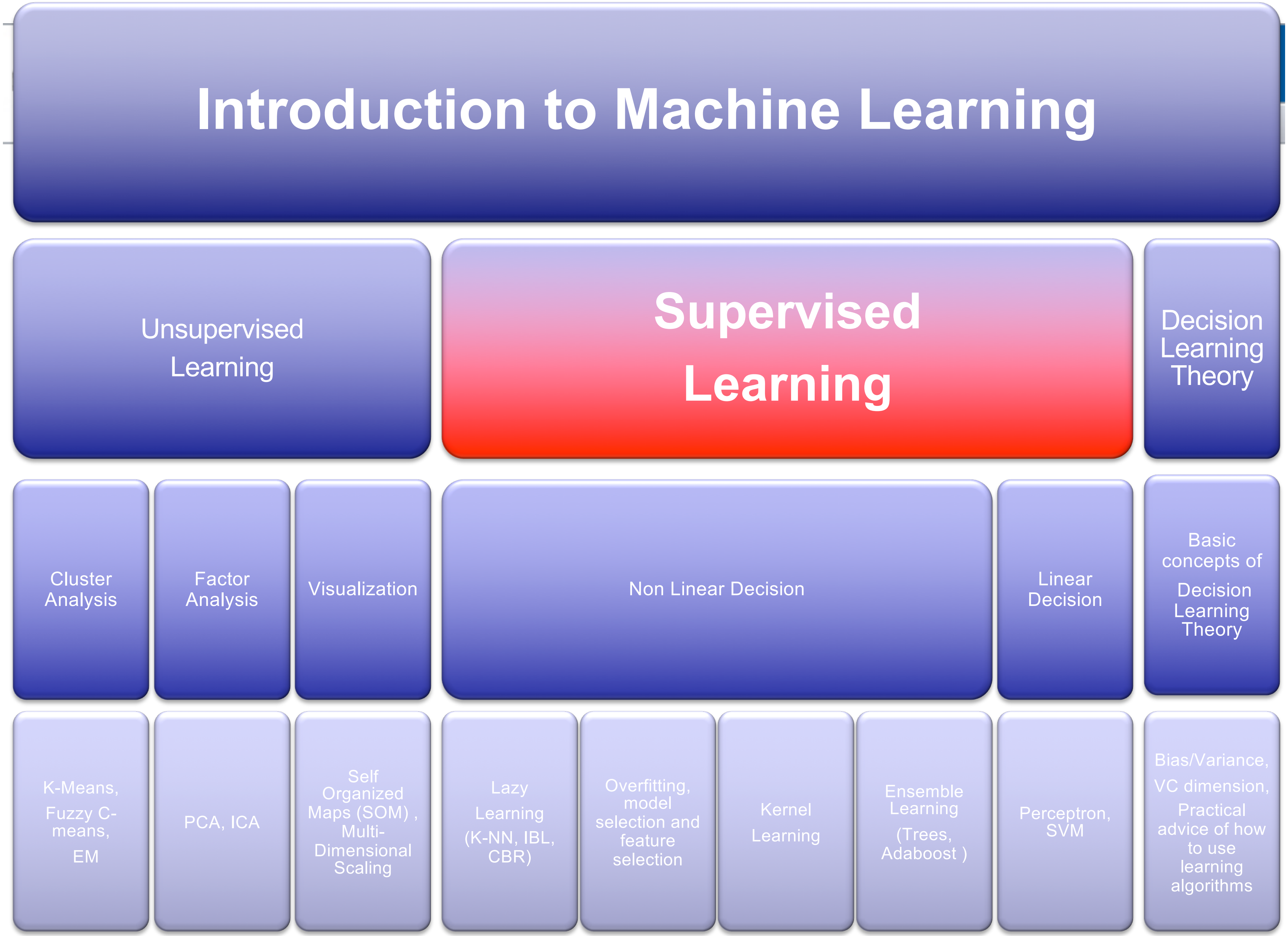
This slides partially come from Oriol Pujol. He has been teaching this course during 4 years and Machine Learning is one of his passions.


Introduction to Machine Learning
Unsupervised Learning
Supervised Learning
Decision Learning Theory
Cluster Analysis
Factor Analysis
Visualization
Non Linear Decision
Linear Decision
Basic concepts of Decision Learning Theory
K-Means, Fuzzy C-means, EM
PCA, ICA
Self Organized Maps (SOM) , Multi-Dimensional Scaling
Lazy Learning (K-NN, IBL, CBR)
Overfitting, model selection and feature selection
Kernel Learning
Ensemble Learning (Trees, Adaboost )
Perceptron, SVM
Bias/Variance, VC dimension, Practical advice of how to use learning algorithms

# Contents

# What is supervised learning?

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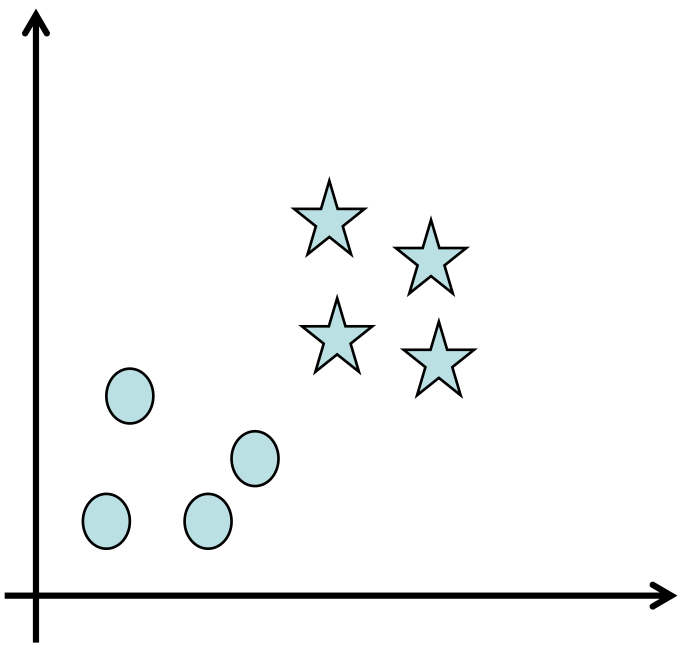
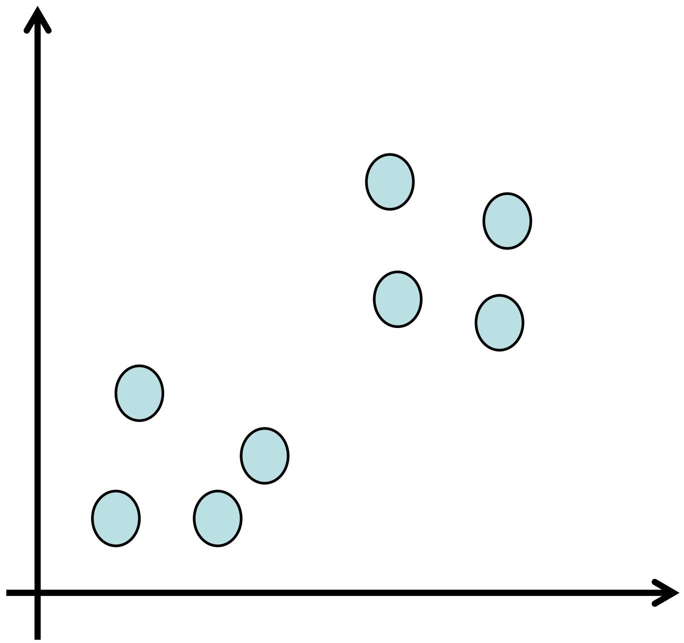
## Supervised



## Unsupervised



# What is supervised learning?

Improve the performance of a software system, based on previous experience

**Tasks**:

- **prediction**: phone and credit card fraud, medical diagnosis, document retrieval,
- **understanding**: market basks, discovering astronomical features
- **control**: flying helicopters, playing backgammon

# Key elements for machine learning

Machine learning is used when:

- There is a pattern
- We can not pin it down mathematically
- We have data on it

Which is the most important of the three?

That's why we also call it **Learning from data**

# What is Machine Learning?

Improve the performance of a software system, based on previous experience:

- **prediction**: **supervised learning**: given *(x, y)* pairs, find a mapping from a new *x* to a new *y*, e.g., regression, classification
- **understanding**: **unsupervised learning**: given a set of x, find something interesting or useful about their structure, e.g. density estimation, clustering, dimensionality reduction
- **control**: **reinforcement learning**: given an external system upon which you can exert control action *a* and receive percepts, *p*, a reward signal *r* indicating good performance, find a mapping from $P \rightarrow A$ that maximizes some long-term measure of *r*

# Generalization in Supervised Learning

We want to find a model that will perform the best on future examples

- We don’t know what the future data will be
- We have **some past data**
- We **hope** that future data will remember past data in a way that while let us use the past data to construct a model that will perform well in the future

# Framing the problem

Humans have to do a lot of work, up front, to set up a machine learning problem

- What do you want to predict?
- What kind of data can you get?
- What is the relative costs of different types of errors?
- How does the available data relate to future data?

# An introductory example

# An example

**Suppose you want to know which grade I may obtain at the end this course**

If you know information (students record) about people who passed this course (data *x*), and their performance (label *y*), then, given your own record you may ask the system to predict your grade based on the previous experience and the power of the learning algorithm.

# An example

| Av. math grade | Grade in ML |
|---|---|
| 5.0 | 4.2 |
| 6.2 | 5.9 |
| 7.4 | 8.1 |
| $\vdots$ | $\vdots$ |

Supervised learning:
Given the "right" answer for each example in de data.

Regression problem:
Predict a real-value output.

## Notation

**Input (features):** $\mathbf{x} \in \mathbf{R}^d$ (student's record)
**Output (labels):** $y \in \mathbf{R}$ (actual grade in ML)
**Data:** Examples of inputs and output pairs: $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

# Dataset jargon

We will usually use column-wise notation for each sample.

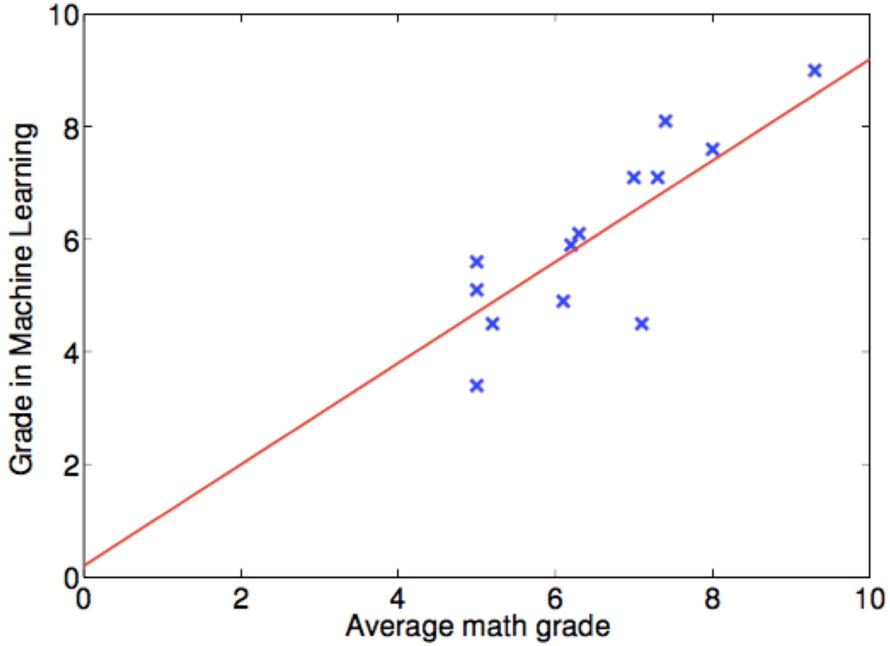
## Common jargon:

**Rows:** features/ attributes/ dimensions.
**Columns:** instances/ examples/ samples.
**The feature to be predicted:** target/ outcome/ response/ label/ dependent variable.
**The other features:** independent variables/ covariates/ predictors/ regressors.

## According to the type of data, we can talk about:

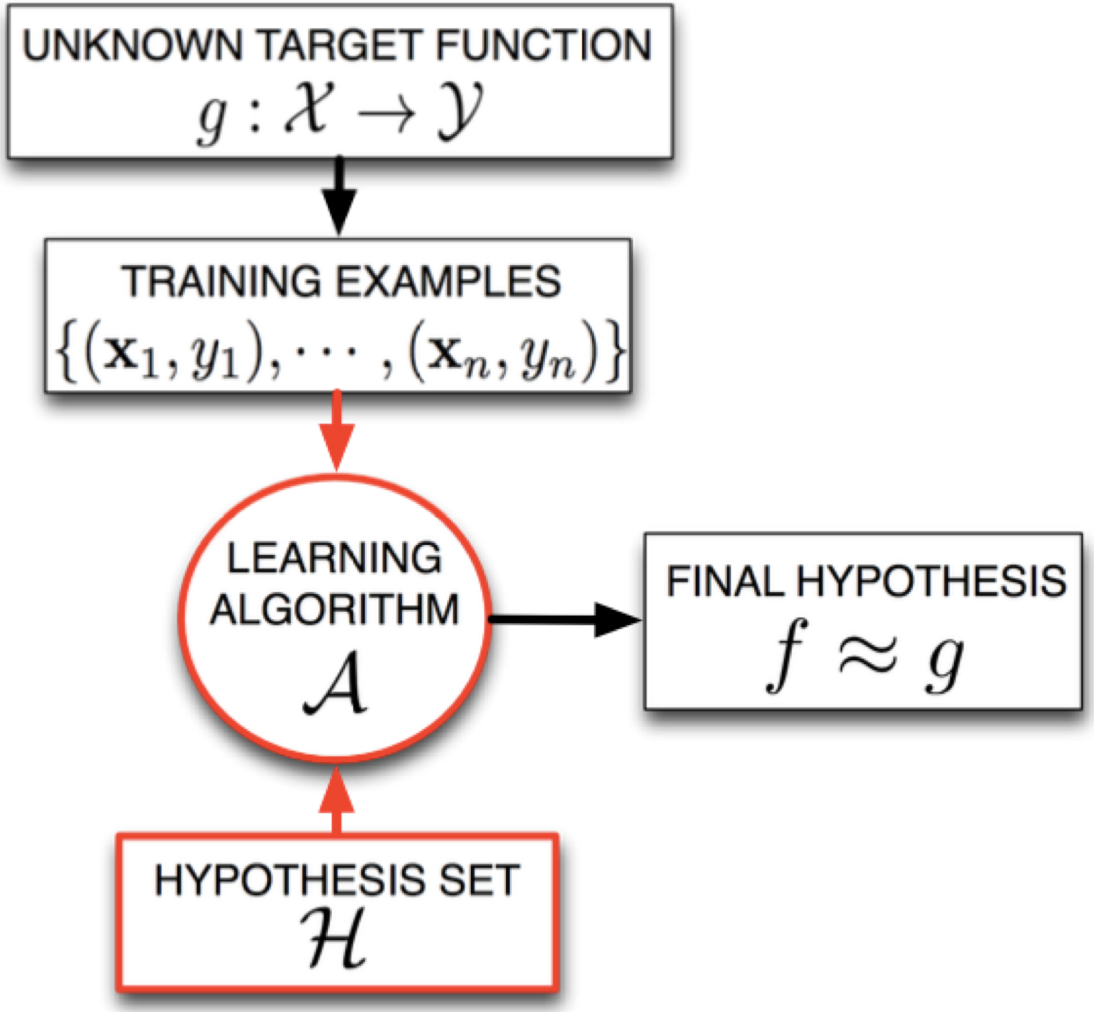
- iid (independent identically distributed) vectors
- Time series (dependent vectors)
- Images (matrices)
- Variable-size non-vector data (e.g. strings, trees, graphs, text)
- Objects (e.g. within a relational schema)

# An example




**Hypothesis:** $f : \mathbf{R}^d \rightarrow \mathbf{R}$ A model that maps from the input data to the output label, e.g. $f(x) = 0.9x + 0.5$
**Learning algorithm:** The process for selecting the most appropriate hypothesis from a hypothesis set $\mathcal{H}$, e.g. the set of linear models $\mathcal{H}(w_0, w_1) \equiv w_1 x + w_0$, where $(w_0, w_1)$ are called parameters.

# The supervised classification problem



# Elements of the supervised problem

**Data:**

Training: $\{(\mathbf{x}_1, y_1) \ldots (\mathbf{x}_N, y_N)\}$; $\quad (\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$

where

$\mathbf{x}$ is the feature data set.

$\mathbf{y}$ is the target output / label.

**Model:**

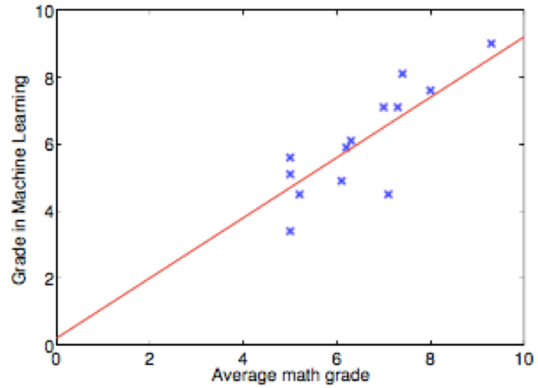
- Hypothesis set: The set of possible / candidate models, $\mathcal{H}$.
- Learning algorithm: The method for selecting the most appropriate model candidate ($f$) with respect to some quality function (e.g. model accuracy)

**Output:** The selected model, $f \in \mathcal{H}$.

# 1st supervised learning model: Linear regression

**Univariate linear regression hypotheses set**

$$\mathcal{H}(w_0, w_1) \equiv w_1 x + w_0.$$




**Learning process idea:**

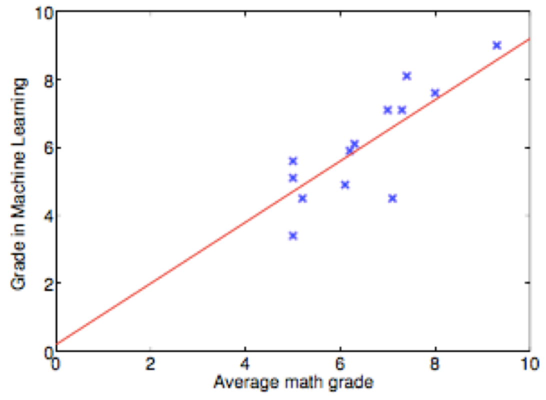
We want to find the model defined by the parameters $(w_0, w_1)$ so that our prediction $f(x_i; w_0, w_1)$ on sample $x_i$ is as close as possible to $y_i$. This is, the "distance" between $f(x_i; w_0, w_1)$ and $y_i$ is minimum for all elements in the training set.

$$\underset{w_0, w_1}{\text{minimize}} \; \frac{1}{N} \sum_{i=1}^{N} \left(f(x_i; w_0, w_1) - y_i\right)^2$$

# 1st supervised learning model: Linear regression

**Univariate linear regression hypotheses set**

$\mathcal{H}(w_0, w_1) \equiv w_1 x + w_0.$




**The last ingredient:**

**The cost function/ loss function/ error measure:**

$$\underset{w_0, w_1}{\text{minimize}}\; J(w_0, w_1)$$

# Putting all the elements together

**Hypothesis**:

$$f(x, w) = w_1 x + w_0$$

**Parameters**:

$$w = (w_0, w_1)^T$$

**Cost function**:

$$\mathcal{J}(w_0, w_1) = \frac{1}{N}\sum_{i=1}^{N}(f(x_i; w_0, w_1) - y_i)^2$$

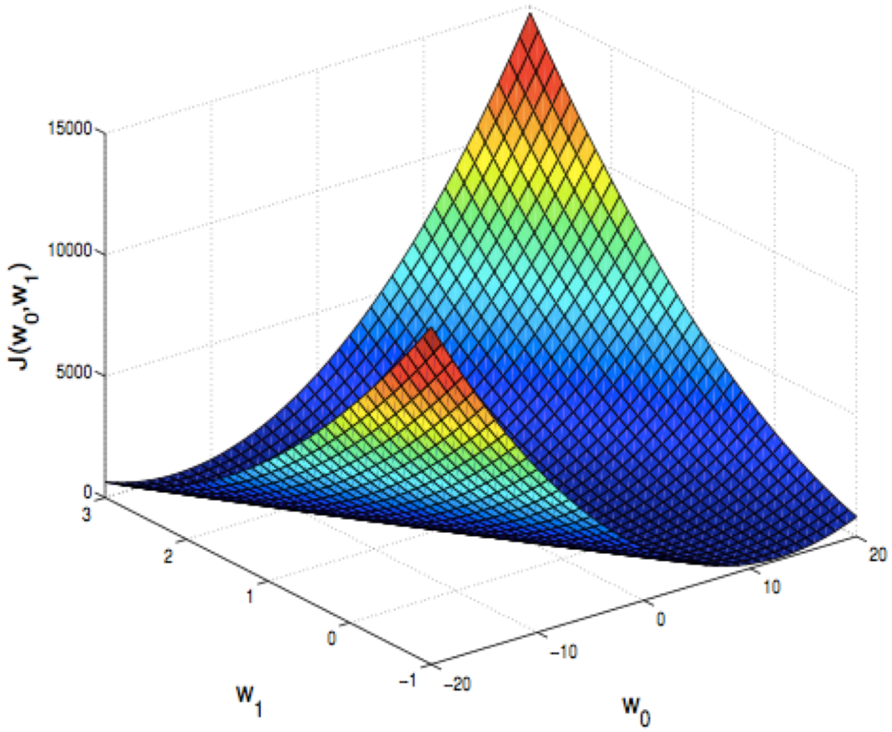
**Goal**:

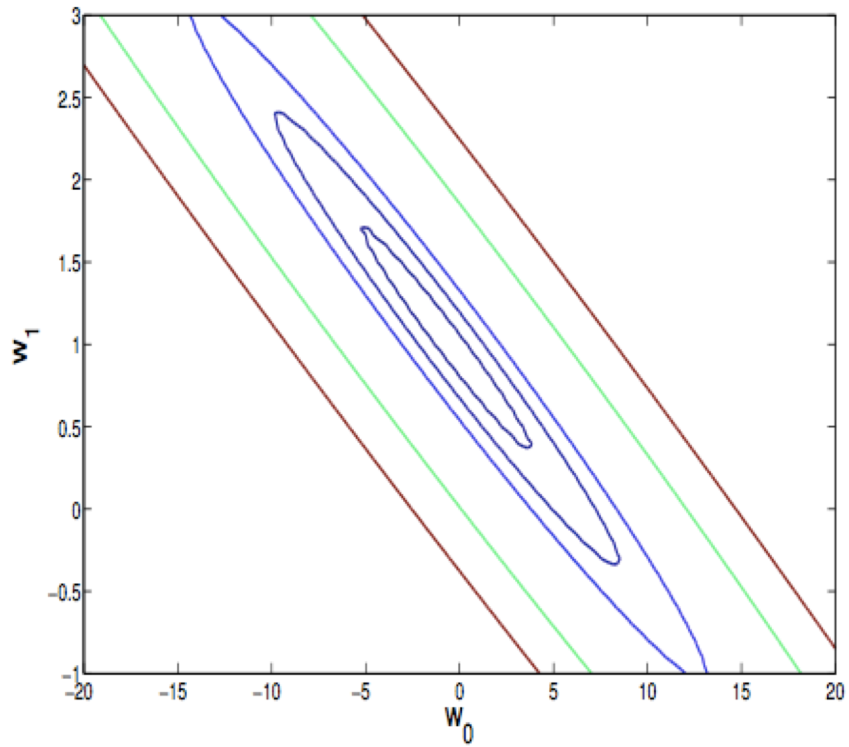
$$\underset{w_0, w_1}{minimize}\ \mathcal{J}(w_0, w_1)$$

# Traveling across the parameter space

## Descent optimization methods

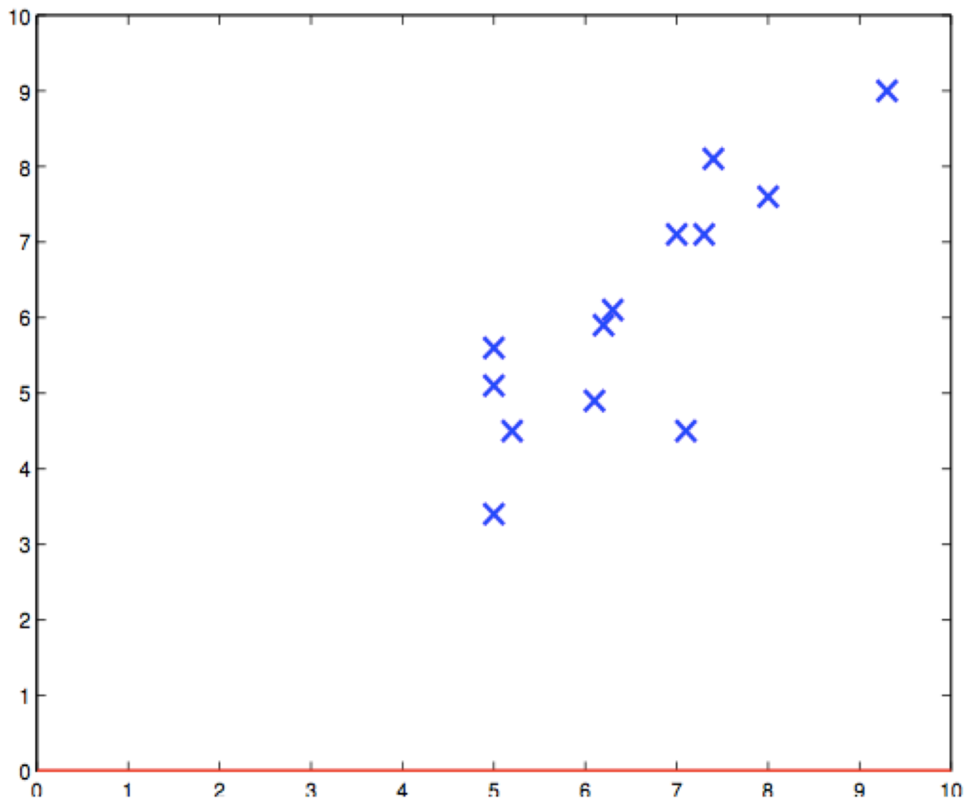
# Visualizing the parameter space



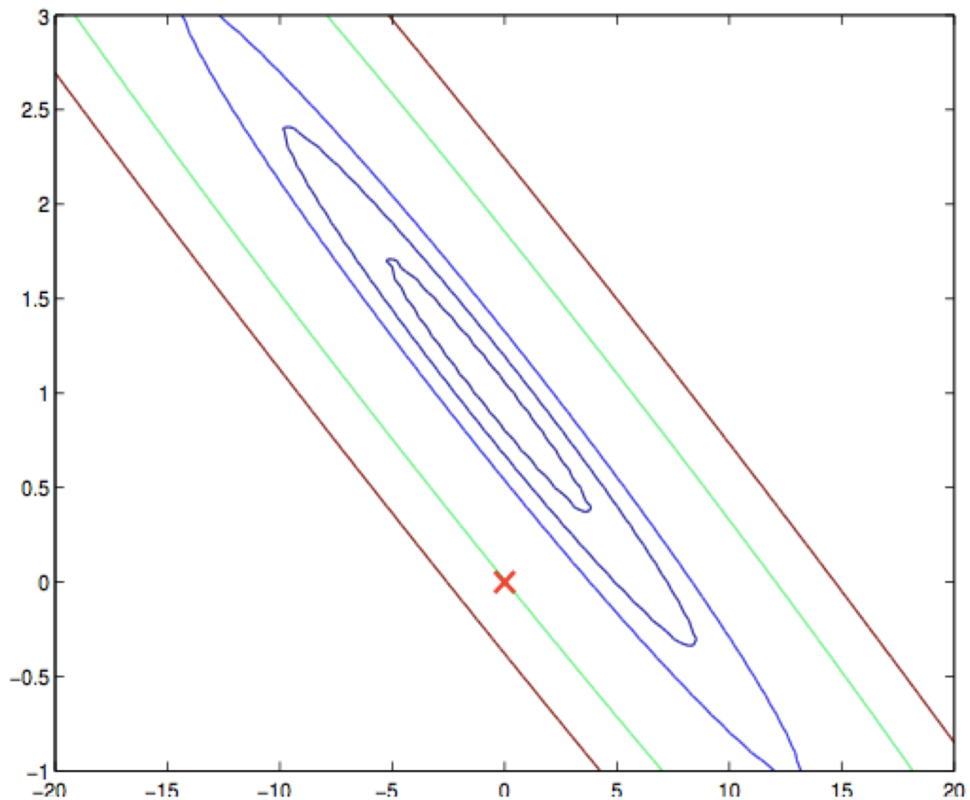



# Visualizing the parameter space

$f_{\mathbf{w}}(x)$

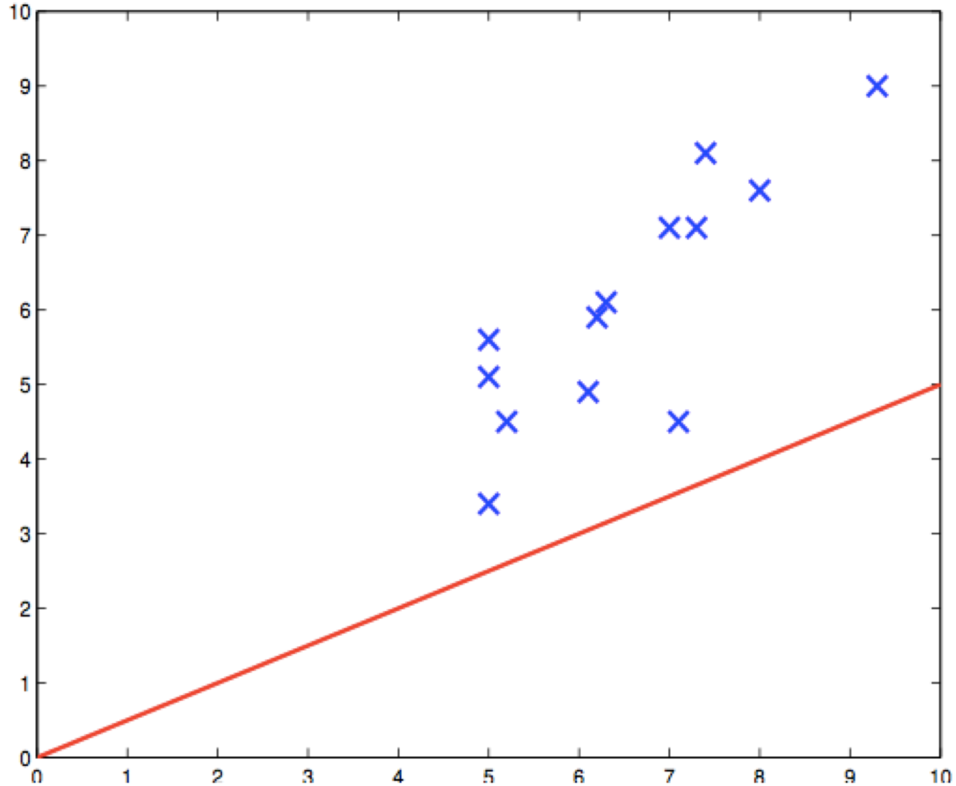


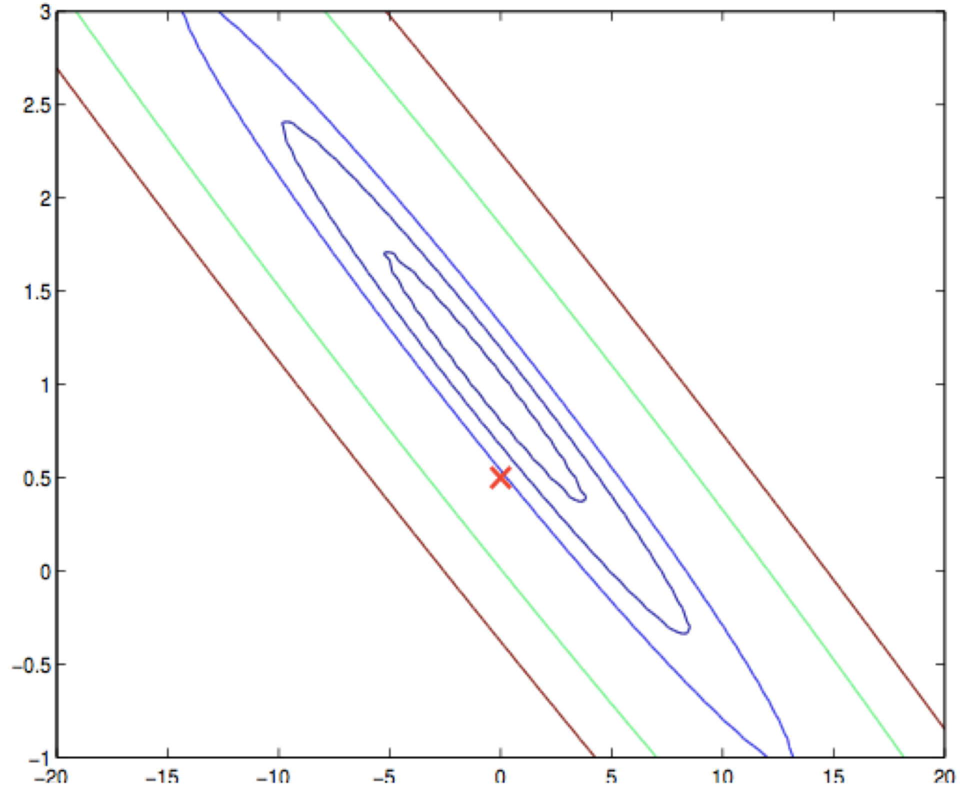

$J(\mathbf{w})$




$$w_0 = 0, \; w_1 = 0$$

# Visualizing the parameter space

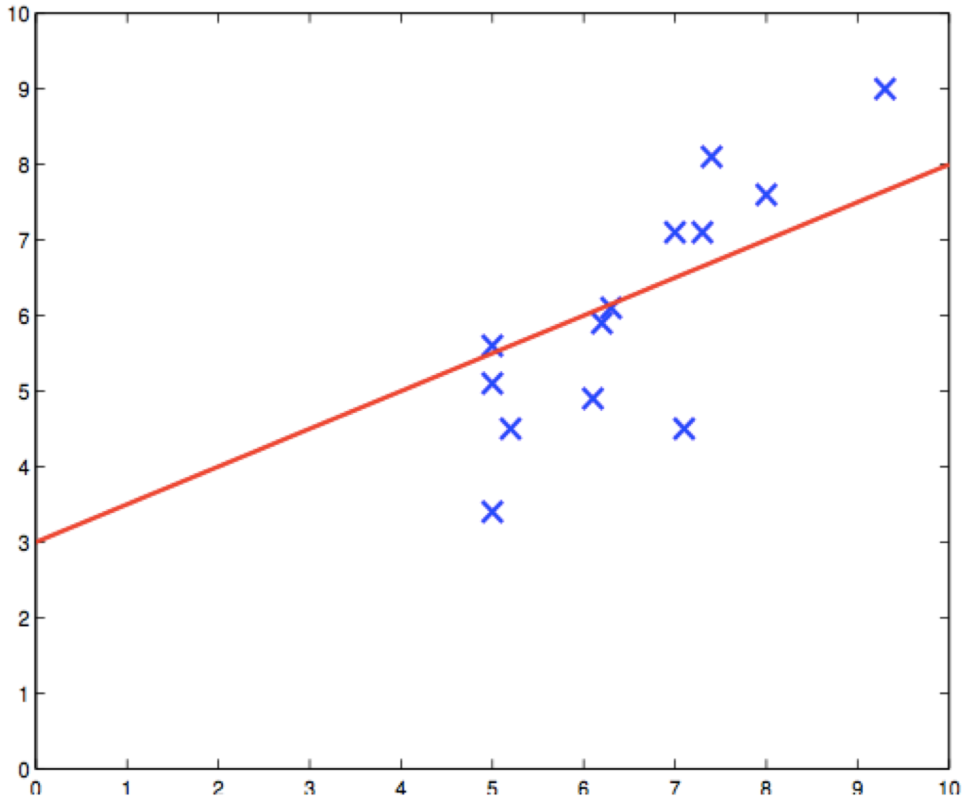


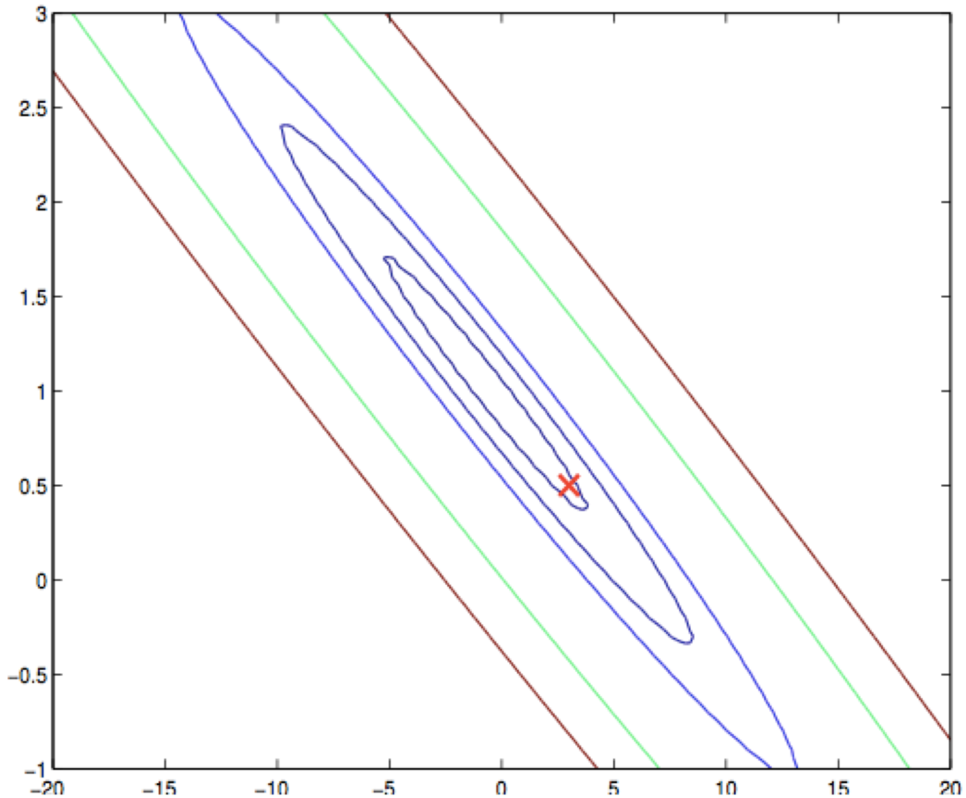

$$w_0 = 0, \; w_1 = 0.5$$

# Visualizing the parameter space

$f_{\mathbf{w}}(x)$



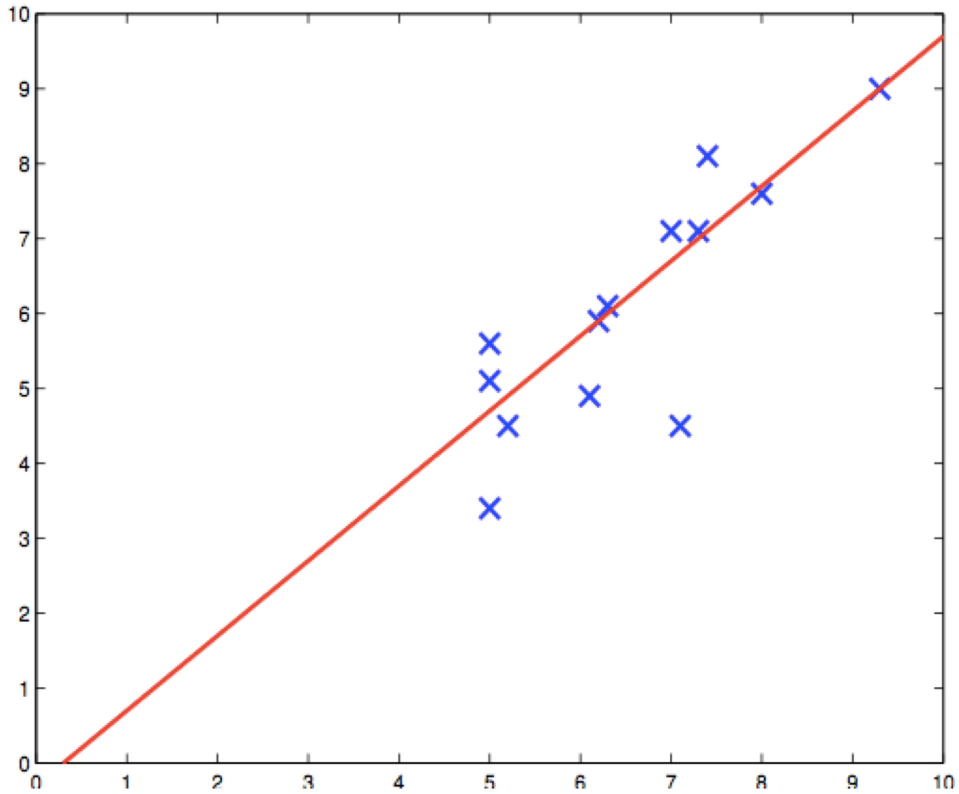

$J(\mathbf{w})$

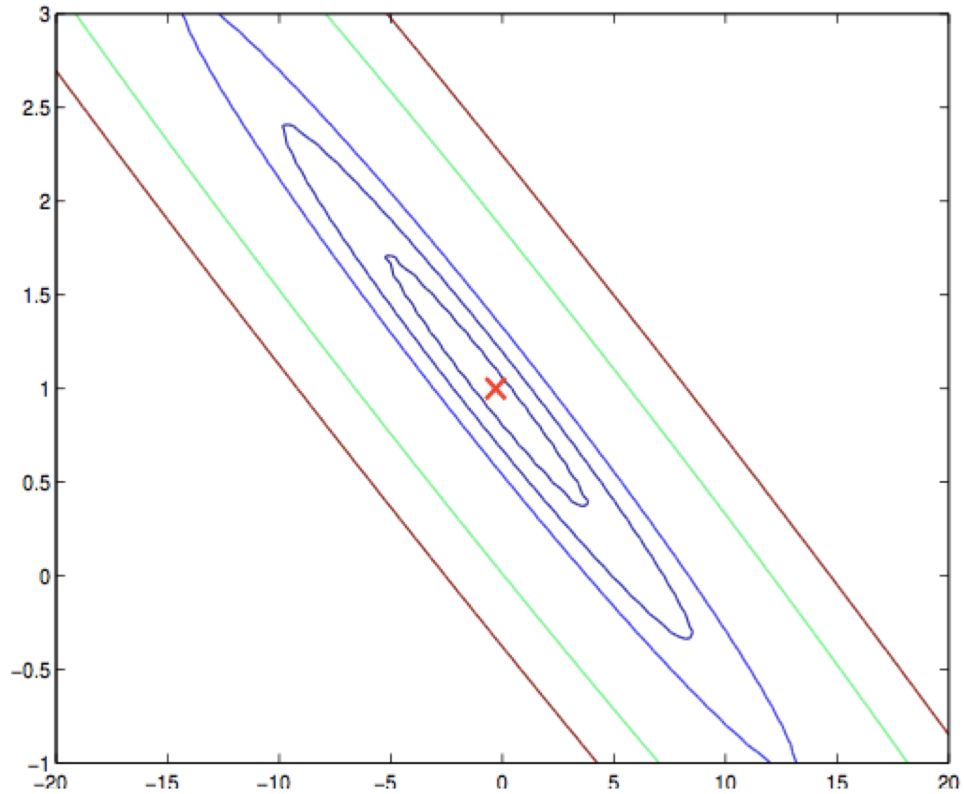



$$w_0 = 3, \; w_1 = 0.5$$

# Visualizing the parameter space

$f_{\mathbf{w}}(x)$ $J(\mathbf{w})$





$w_0 = -0.3, \; w_1 = 1$

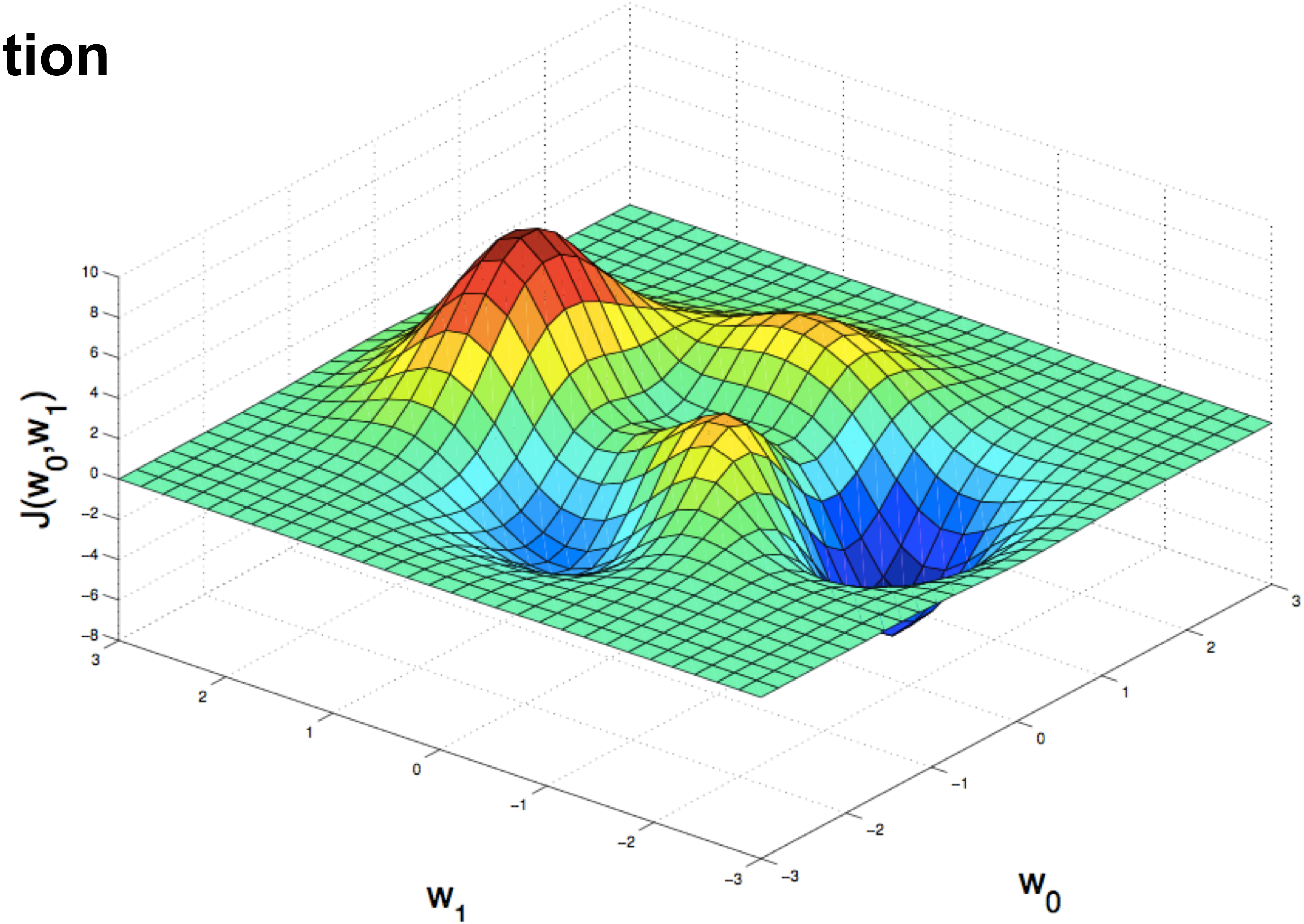
# Traveling across the parameter space

**Question**:
How do we find the minimum in an automated way?

**A basic technique:**

1. Start with some starting point (guess) $(w_0^{(0)}, w_1^{(0)})$.
2. Change the parameters so that we reduce the cost function $J(w_0^{(k+1)}, w_1^{(k+1)}) < J(w_0^{(k)}, w_1^{(k)})$
3. Repeat (2) until the cost function is not reduced anymore.

## Intuition



## With descent methods

**Input**: given a starting point $x \in \mathbf{dom}\ f$
**Output**:
**while** *stopping criterion is not satisfied:* **do**
    (a) Determine a descent direction $\Delta x$;
    [(b) *Line search.* Choose a step size $t > 0$];
    (c) *Update.* $x := x + t\Delta x$;
**end**

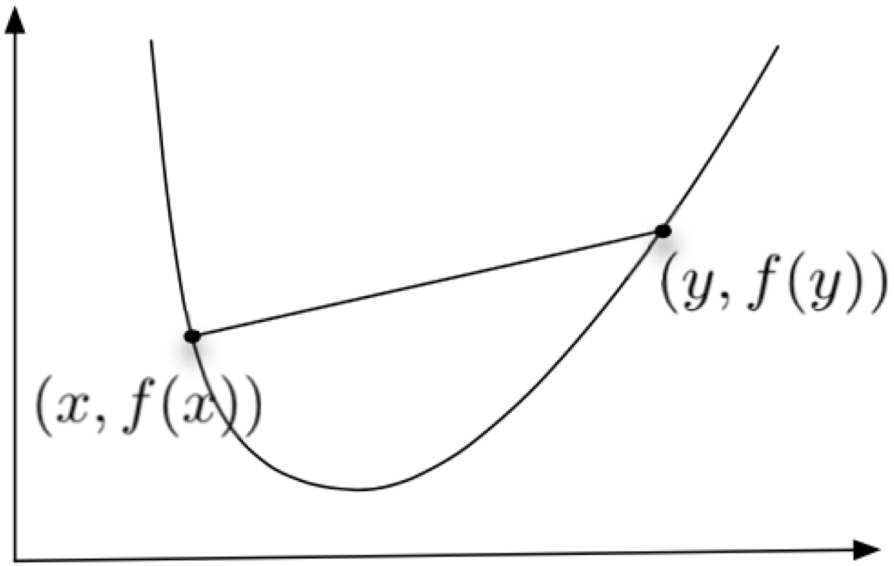
**Algorithm 1:** General descent method

# With descent methods. Previous Concepts.

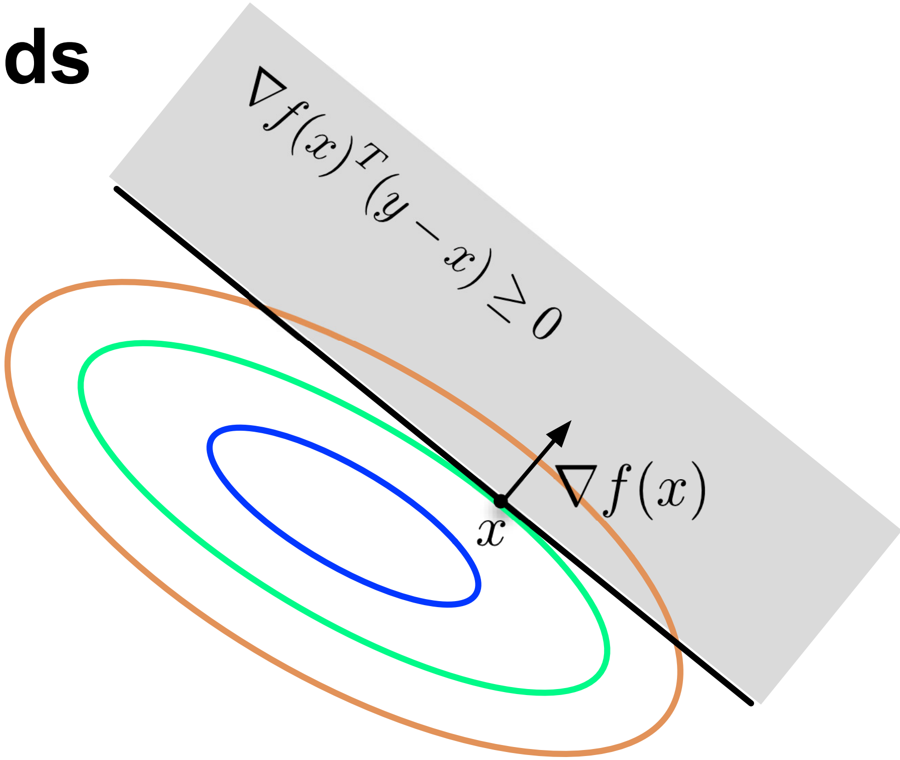
## Previous concepts

**Definition** A function $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is *convex* if $\mathbf{dom}\, f$ is a convex set and if for all $x, y \in \mathbf{dom}\, f$, and $\theta$ with $0 \leqslant \theta \leqslant 1$, we have

$$f(\theta x + (1-\theta)y) \leqslant \theta f(x) + (1-\theta) f(y).$$



## With descent methods

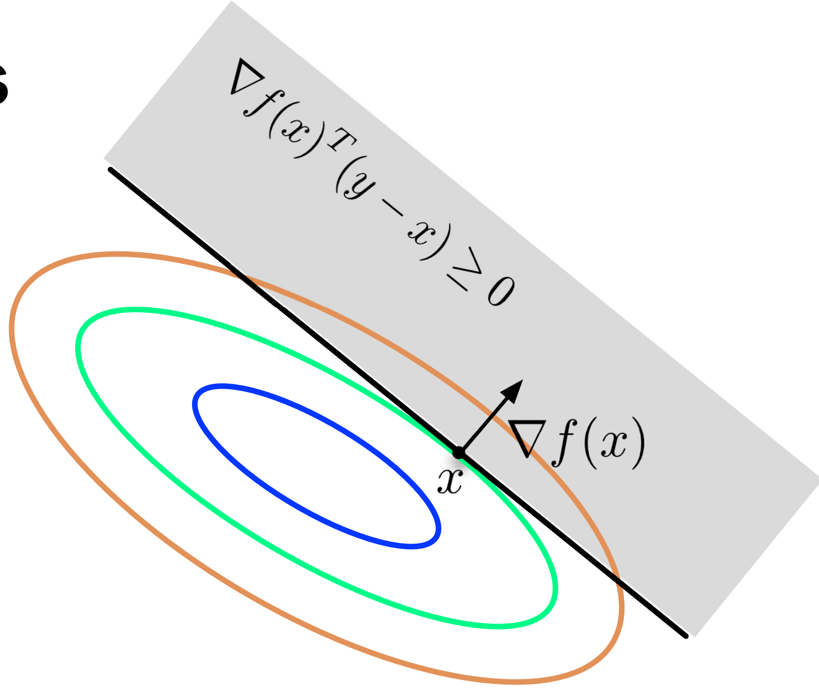



### Previous concepts

A differentiable function $f : \mathbf{R}^n \to \mathbf{R}$ is *convex* if and only if **dom** $f$ is convex and

$$f(y) \geqslant f(x) + \nabla f(x)^T(y-x), \quad \forall x, y \in \textbf{dom } f.$$

## With descent methods




A descent direction must satisfy (necessary but not sufficient):

$$\nabla f(x)^T \Delta x < 0.$$

A natural choice is to select the steepest descent direction given by

$$\Delta x = -\nabla f(x).$$

# Gradient/Steepest Descent

**Input**: given a starting point $x \in \mathbf{dom}\ f$
**Output**:
**while** *stopping criterion is not satisfied:* **do**
 (a) Determine a descent direction $\Delta x = -\nabla f(x)$;
 [(b) *Line search.* Choose a step size $t > 0$];
 (c) *Update.* $x := x + t\Delta x$;
**end**

**Algorithm 2:** Gradient descent method

# Steepest descent implementation

**Hypothesis**:

$$f(x, w) = w_0 + w_1 x$$

**Cost function**:

$$\mathcal{J}(w_0, w_1) = \frac{1}{2N} \sum_{i=1}^{N} (f(x_i; w_0, w_1) - y_i)^2$$

**Gradient**:

$$\nabla J(\mathbf{w}) = \left(\frac{\partial J}{\partial w_0}, \frac{\partial J}{\partial w_1}\right)^T$$

$$\frac{\partial J}{\partial w_0} = \frac{1}{N} \sum_{i=1}^{N} (w_0 + w_1 x_i - y_i) 1$$

$$\frac{\partial J}{\partial w_1} = \frac{1}{N} \sum_{i=1}^{N} (w_0 + w_1 x_i - y_i) x_i$$

# Steepest descent implementation

**Input**: given a starting point $\mathbf{w} = (-10, -10)$, $t = 0.001, \tau = 1000$
**Output**: model $\mathbf{w}$
**for** $k = 1 : \tau$ **do**

$$w_0^{(k+1)} := w_0^{(k)} - t\frac{1}{N}\sum_{i=1}^{N}(w_0^{(k)} + w_1^{(k)}x_i - y_i)1;$$

$$w_1^{(k+1)} := w_1^{(k)} - t\frac{1}{N}\sum_{i=1}^{N}(w_0^{(k)} + w_1^{(k)}x_i - y_i)x_i;$$

**end**

# Matrix notation

**Hypothesis:**

$$f(x; w) = w_0 + w_1 x = \begin{pmatrix} 1 & x \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \end{pmatrix} = \begin{pmatrix} 1 & x \end{pmatrix} \mathbf{w} = \tilde{\mathbf{x}}^T \mathbf{w}$$

**Cost function :**

$$J(w_0, w_1) = \frac{1}{N} \sum_{i=1}^{N} (f(x_i; w_0, w_1) - y_i)^2$$

$$= \frac{1}{N} \sum_{i=1}^{N} (\tilde{\mathbf{x}}_i^T \mathbf{w} - y_i)^2$$

$$= \frac{1}{N} (\tilde{\mathbf{X}}^T \mathbf{w} - \mathbf{y})^T (\tilde{\mathbf{X}}^T \mathbf{w} - \mathbf{y})$$

where

$$\tilde{\mathbf{X}} = \begin{pmatrix} \tilde{\mathbf{x}}_1 & \tilde{\mathbf{x}}_2 & \cdots & \tilde{\mathbf{x}}_N \end{pmatrix} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_N \end{pmatrix}$$

# Steepest decent implementation

## In matrix notation

**Hypothesis:**

$$f(x;w) = \tilde{\mathbf{x}}^T \mathbf{w}$$

**Cost function :**

$$J(\mathbf{w}) = \frac{1}{2N}(\tilde{\mathbf{X}}^T\mathbf{w} - \mathbf{y})^T(\tilde{\mathbf{X}}^T\mathbf{w} - \mathbf{y})$$

**Gradient :**

$$\nabla J(\mathbf{w}) = \frac{1}{N}\tilde{\mathbf{X}}(\tilde{\mathbf{X}}^T\mathbf{w} - \mathbf{y})$$

# Application of the learning model

# Application of the learning model

### Training

We are given a dataset $\mathcal{D}$ which we use to learn our model parameters, e.g. the parameters of the linear regressor.

### Exploitation

Apply the learned model to new data and **hope** it predicts correctly.

# A 1st evaluation of the learning model

**But … we want to know aproximately how well it will perform during the exploitation step! What to do?**

### The simplest evaluation strategy: Simulate exploitation data.

We are given a dataset $\mathcal{D}$ and it is divided in two sets

$$\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{test}$$

### Training

Use $\mathcal{D}_{train}$ to learn the model.

### Evaluation

Use $\mathcal{D}_{test}$ to compute the performance of the method.

### Exploitation

Apply the model to new data and **hope** it predicts correctly.

# A 1st evaluation of the learning model

**Suppose that we have two different models. We want to select the one that has a better performance during the exploitation step. But … we don't have exploitation data to evaluate on? What to do?**

### Simulate exploitation data.

We are given a dataset $\mathcal{D}$ and it is divided in two sets

$$\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{validation}$$

### Training

Use $\mathcal{D}_{train}$ to learn both models.

### Evaluation

Use $\mathcal{D}_{validation}$ to decide which of the two models better adapts to our problem.

Apply the selected model to new data and **hope** it predicts correctly.

# A 1st evaluation of the learning model

**But … I want to know the expected performance of the best method!!! What to do?**

### Simulate exploitation data.

We are given a dataset $\mathcal{D}$ and it is divided in three sets

$$\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{validation} \cup \mathcal{D}_{test}$$

### Training and model selection

Use $\mathcal{D}_{train}$ to learn both models. Use $\mathcal{D}_{validation}$ to decide which of the two models better adapts to our problem.

### Evaluation

Use $\mathcal{D}_{test}$ to compute the performance of the selected method.

Apply the selected model to new data and **hope** it predicts correctly.

# A whirlwind tour on machine learning terms

# Basic concepts of Machine Learning

- **How do I learn a simple Gaussian?** Probability, random variables, distributions; estimation, convergence and asymptotics, confidence interval
- **How do I learn a mixture of Gaussians (MoG)?** Likelihood, Expectation-Maximization (EM); generalization, model selection, cross-validation; k-means, Hidden Markov odels (HMM)
- **How do I learn any density?** Parametric vs. non-Parametric estimation, Sobolev and other functional spaces; *l*-2 error; Kernel density estimation (KDE), optimal kernel, KDE theory

# Basic concepts of Machine Learning

- **How do I predict a continuous variable (regression)?** Linear regression, regularization, ridge regression, and LASSO; local linear regression; conditional density estimation.
- **How do I predict a discrete variable (classification)?** Bayes classifier, naive Bayes, generative vs. discriminative; perceptron, weight decay, linear support vector machine; nearest neighbor classifier and theory

General theory and model frameworks of Machine Learning

- **Which loss function should I use?** Maximum likelihood estimation theory; $l$-2 estimation; Bayessian estimation; minimax and decision theory, Bayesianism vs frequentism
- **Which model should I use?** AIC and BIC; Vapnik-Chervonenskis theory; cross-validation theory; bootstrapping; Probably Approximately Correct (PAC) theory; Hoeffding-derived bounds.

# Basic concepts of Machine Learning

General theory and model frameworks of Machine Learning

- **How can I learn fancier (combined) models?** Ensemble learning theory; boosting; bagging; stacking.
- **How can I learn fancier (nonlinear) models?** Generalized linear models, logistic regression; Kolmogorov theorem, generalized additive models; kernelization, reproducing kernel Hilbert spaces, non-linear SVM, Gaussian process regression
- **How can I learn fancier (compositional) models?** Recursive models, decision trees, hierarchical clustering; neural networks, back propagation, deep belief networks; graphical models, mixtures of HMMs, conditional random fields, max-margin Markov networks; log-linear models; grammars

Further common machine learning problems and solutions

- **How do I reduce or relate features?** Feature selection vs dimensionality reduction, wrapper methods for feature selection; causality vs correlation, partial correlation, Bayes net structure learning
- **How do I create new features?** principal component analysis (PCA), independent component analysis (ICA), multidimensional scaling (MDS), manifold learning, supervised dimensionality reduction, metric learning
- **How do I reduce or relate the data?** Clustering, bi-clustering, constrained clustering; association rules and market basket analysis; ranking/ordinal regression; link analysis; relational data

Further common machine learning problems and solutions

- **How do I treat time series?** ARMA; Kalman filter and stat-space models, particle filter; functional data analysis; change-point detection; cross-validation for time series
- **How do I treat non-ideal data?** covariate shift; class imbalance; missing data, irregularly sampled data, measurement errors; anomaly detection, robustness

General computational frameworks for machine learning

- **How do I optimize the parameters?** Unconstrained vs constrained/Convex optimization, derivative-free methods, first- and second-order methods, backfitting; natural gradient; bound optimization and EM
- **How do I optimize linear functions?** computational linear algebra, matrix inversion for regression, singular value decomposition (SVD) for dimensionality reduction
- **How do I optimize with constraints?** Convexity, Lagrange multipliers, Karush-Kuhn-Tucker conditions, interior point methods, SMO algorithm for SVM

General computational frameworks for machine learning

- **How do I evaluate deeply-nested sums?** Exact graphical model inference, variational bounds on sums, approximate graphical model inference, expectation propagation
- **How do I evaluate large sums and searches?** Generalized N-body problems (GNP), hierarchical data structures, nearest neighbor search, fast multiple method; Monte Carlo integration, Markov Chain Monte Carlo, Monte Carlo SVD
- **How do I treat even larger problems?** Parallel/distributed EM, parallel/distributed GNP; stochastic subgradient methods, online learning

## Real-world application of machine learning

- **How do I apply all this in the real world?** Overview of the parts of the ML, choosing between the methods to use for each task, prior knowledge and assumptions; exploratory data analysis and information visualization; evaluation and interpretation, using confidence intervals and hypothesis test, ROC curves; where the research problems in ML are

# Course. Introduction to Machine Learning
# Lecture 6. A gentle introduction to Supervised Learning

THE END