Recitation 1

Statistical Learning Theory
Intro to Gradient Descent

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CDS

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Introduction

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Office Hours:
Colin: Mon 1:00PM-2:00PM, Vishakh: Wed 6:00PM-7:00PM

Motivation

In data science, we generally need to **Make a Decision** on a problem.
To do this, we need to understand

- The setup of the problem
- The possible actions
- The effect of actions
- The evaluation of the results

How do we translate the problem into the language of DS/modeling?

Formalization

The Spaces

$\mathcal{X}$: input space $\mathcal{Y}$: outcome space $\mathcal{A}$: action space

Prediction Function

A **prediction function** f gets an input $x \in \mathcal{X}$ and produces an action $a \in \mathcal{A}$:

$$f : \mathcal{X} \mapsto \mathcal{A}$$

Loss Function

A **loss function** $\ell(a, y)$ evaluates an action $a \in \mathcal{A}$ in the context of an outcome $y \in \mathcal{Y}$:

$$\ell : \mathcal{A} \times \mathcal{Y} \mapsto \mathbb{R}$$

Risk Function

- Given a loss function ℓ, how can we evaluate the "average performance" of a prediction function f?
- To do so, we need to first assume that there is a **data generating distribution** $\mathcal{P}_{x,y}$.
- Then the expected loss of f on $\mathcal{P}_{x,y}$ will reflect the notion of "average preformance".

Definition

The **risk** of a prediction function $f : \mathcal{X} \mapsto \mathcal{A}$ is

$$R(f) = \mathbb{E}\ell(f(x), y)$$

It is the expected loss of f on a new sample (x, y) drawn from $\mathcal{P}_{X,Y}$.

Finding 'best' function

Definition

$\mathfrak{F}$ is the family of functions we restrict our model to be.
Example: Linear, quadratic, decision tree, two layer neural-net...

Definition

$f_{\mathfrak{F}}$ is 'best' function one can obtain within $\mathfrak{F}$.

Definition

$\hat{f}_n$ is the 'best' function one can obtain using the data given.

Definition

$\tilde{f}_n$ is the function actually obtained using the data given.

The Bayes Prediction Function

Definition

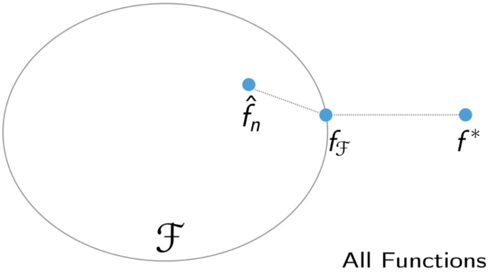
A **Bayes prediction function** $f^* : \mathcal{X} \mapsto \mathcal{Y}$ is a function that achieves the *minimal risk* among all possible functions:

$$f^* \in \arg\min_f R(f),$$

where the minimum is taken from all functions that maps from $\mathcal{X}$ to $\mathcal{A}$.

The risk of a Bayes function is called **Bayes risk**.

Error Decomposition



Example

Error Decomposition

- Approximation Error
  - Caused by the choice of family of functions or capacity of the model.
  - Expand the capacity of the model.
- Estimation Error
  - Caused by finite number of data
  - Obtain more data/add regularizer
- Optimization Error
  - Caused by not able to find the best parameters
  - Try different optimization algorithms, learning rates, etc.

Gradient Descent

Motivation:

- Our goal is the find $\hat{f}_n$, the best possible model from given data
- Naive approach: Take gradient of loss function, solve for parameters that gives you 0.
  - Computationally intractable
  - Impossible to compute due to complex function structure
- The optimal parameters for LR: $\hat{\beta} = \left(X^\top X\right)^{-1} X^\top Y$
- When X's dimension reaches the millions, the inverse is essentially intractable.

But we do not need $\hat{f}_n$, a close $\tilde{f}_n$ is good enough for decision making. Therefore, instead of solving for the best parameters, we just need to approximate it well enough.

Gradient Descent

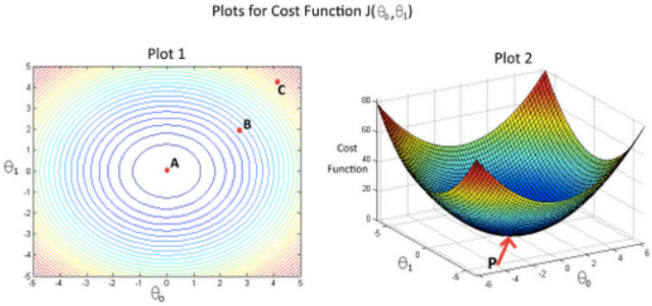
Idea:

- Given any starting parameters, the gradient indicates the direction of local maximal change.
- If we obtain new parameters by moving old parameter along its gradient, the new ones will give smaller loss (if we are careful).
- We can repeat this procedure until we are happy with the result.

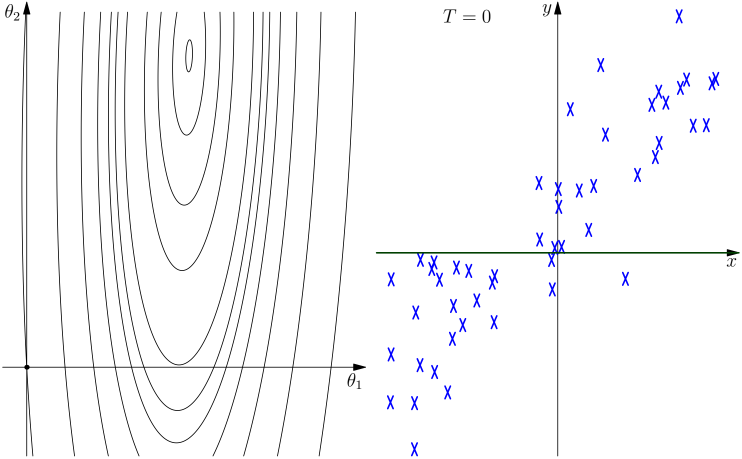
Contour Graphs

Imagine we are solving a simple linear regression problem: $y = \theta_0 + \theta_1 x$ with loss function:

$$J(\theta_0, \theta_1) = \sum^{n} (y_i - (\theta_0 + \theta_1 x_i))^2$$



Negative Gradient Steps



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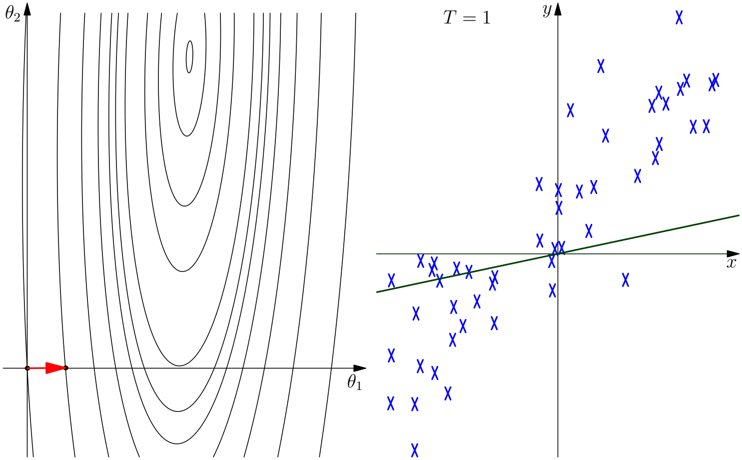

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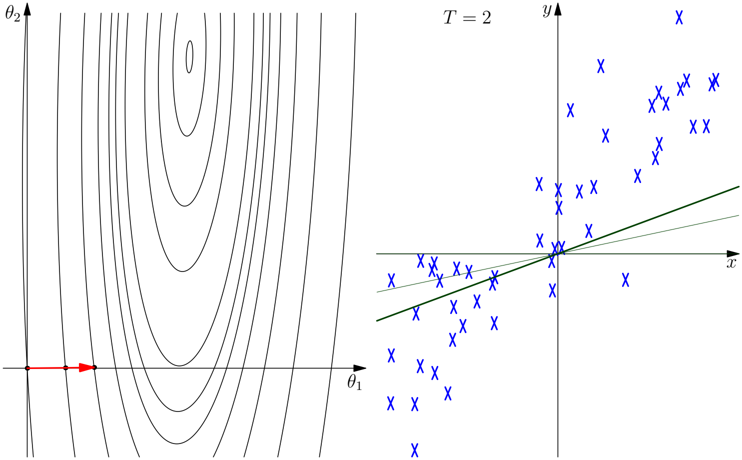

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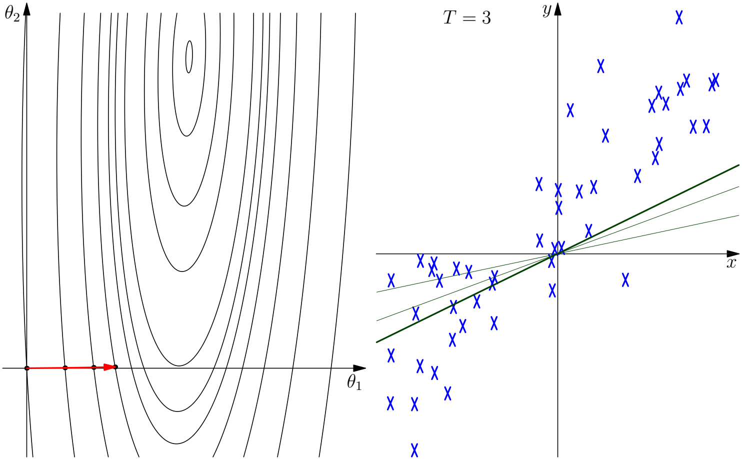

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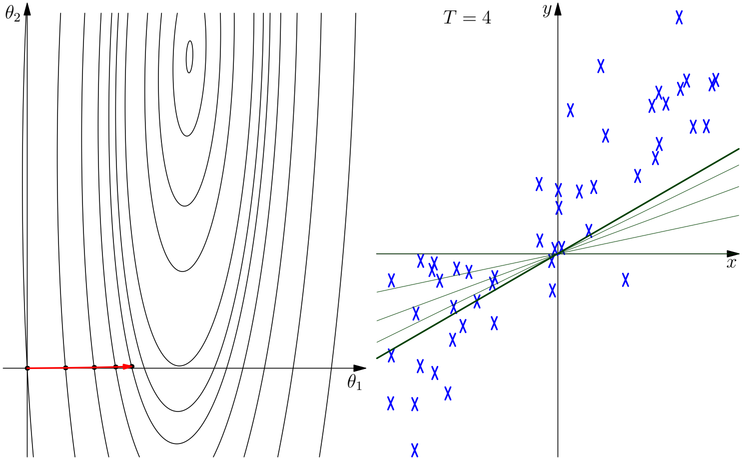

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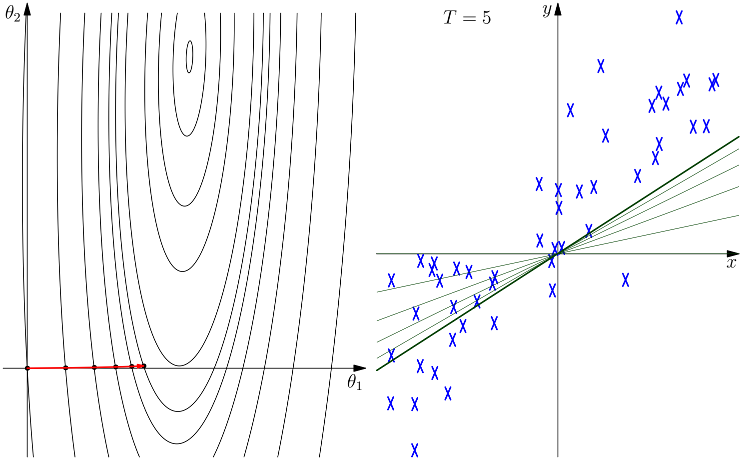

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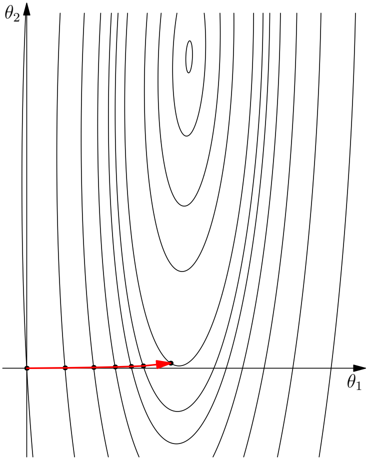

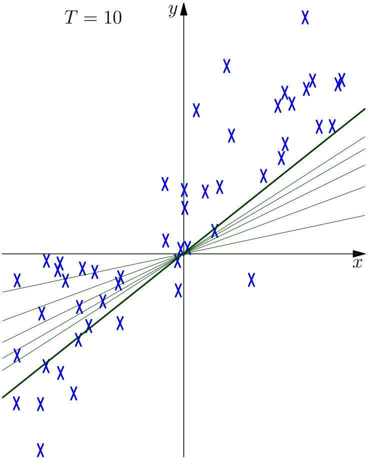

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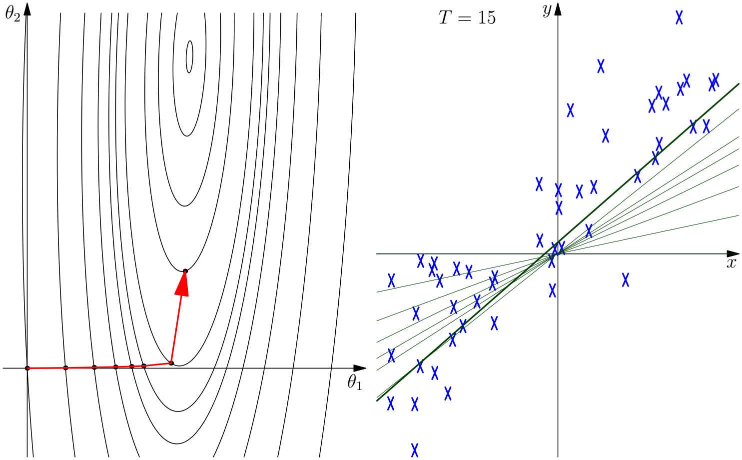

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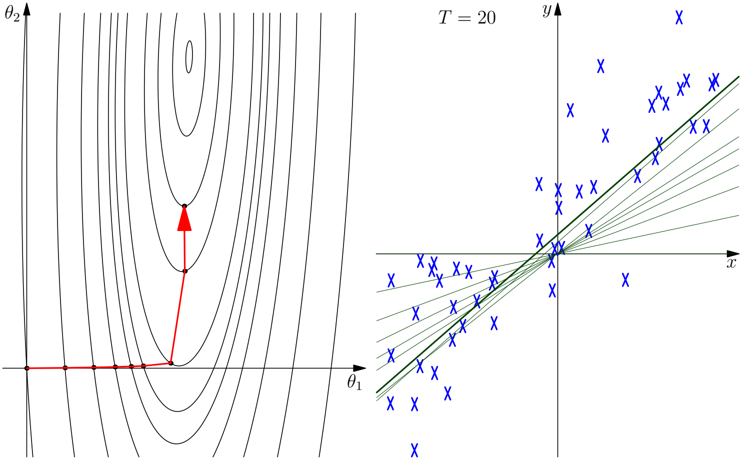

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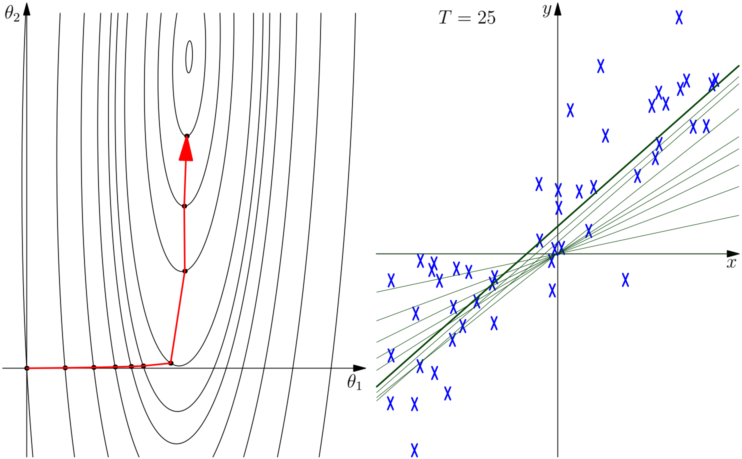

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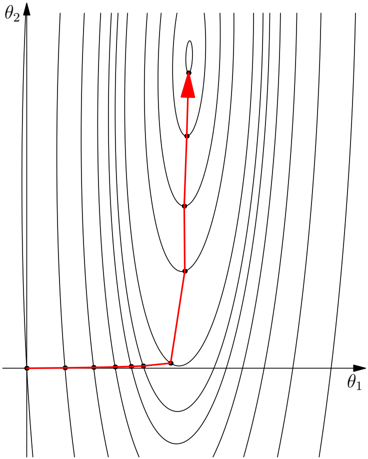

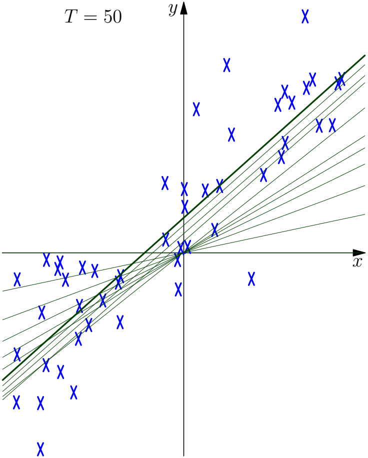

Gradient Descent

Gradient descent Algorithm

- Goal: find $\theta^* = \arg\min_\theta J(\theta)$
- θ^0 :=[initial condition] (can be randomly chosen)
- $i := 0$
- while not [termination condition]:
  - compute $\nabla J(\theta_i)$
  - α :=[choose learning rate at iteration i]
  - $\theta^{i+1} := \theta^i - \alpha \nabla J(\theta_i)$
  - $i := i + 1$
- return θ^i

Things to review

- Calculus
  - Gradients, taking (partial) derivatives
- Linear Algebra
  - Matrix computation, matrix derivatives
  - Example: compute $\frac{\partial x^T A x}{\partial x}$, where A is a matrix and x is a vector