Distributed Optimization for Machine Learning

Lecture 4 - Unconstrained Optimization: Gradient Descent

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Different perspectives of (pre)training AI models

1. Given training data $\{\mathbf{x}\}$, develop a Model $h_{\boldsymbol{\theta}}(\mathbf{x})$
2. Define a Loss Function $L(\boldsymbol{\theta})$ based on the format $\{\mathbf{x}\}$
3. Design an Optimization Algorithm to minimize the loss

This three-step framework – **Model, Loss, and Optimization** - is the fundamental blueprint for almost all of supervised machine learning.

Different perspectives of (pre)training AI models

1. Given training data $\{\mathbf{x}\}$, develop a Model $h_{\boldsymbol{\theta}}(\mathbf{x})$

$\downarrow$

2. Define a Loss Function $L(\boldsymbol{\theta})$ based on the format $\{\mathbf{x}\}$

We will further extend to different data modality and different state-of-the-art (SOTA) models in Theme 3 of the class.

Generic (model-agnostic) optimization

3. Design an Optimization Algorithm to minimize the loss $L(\boldsymbol{\theta})$

In the next few lectures, we will first review some generic (model-agnostic and data-agnostic) **optimization** techniques - which are the fundamental for training almost all types of machine learning and AI models.

[†]Since we first consider data-agnostic optimization, the algorithms are all "batch" algorithms, which use the entire dataset to compute each optimization update.

Differentiable unconstrained minimization

For now on, let's use $\mathbf{x}$ to replace $\boldsymbol{\theta}$ as the optimization variable

$$\begin{array}{ll} \min_{\mathbf{x}} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \mathbb{R}^n \end{array}$$

- f (objective or cost function) is differentiable

Why not solve $\nabla f(\mathbf{x}) = 0$ directly?

For simple functions, we can find the **analytical solution** by solving

$$f(x) = (x-3)^2 \implies \nabla f(x) = 2(x-3) = 0 \implies x = 3.$$

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For AI/ML, this direct approach is usually **impossible** for several reasons:

No closed-form solution

For a deep neural network, $\nabla f(\mathbf{x}) = 0$ is a massive system of highly non-linear, coupled equations. No algebraic formula to solve for $\mathbf{x}$.

Prohibitive computational cost

Even when a closed-form solution exists, it requires computationally infeasible operations, like inverting a massive matrix ($O(n^3)$ cost).

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Local minima & saddle points

Solving $\nabla f(\mathbf{x}) = 0$ finds all *stationary points*, including maxima and saddle points. Iterative algorithms move "downhill" to find a minimum.

Iterative descent algorithms

Start with a point $\mathbf{x}^0$, and construct a sequence $\{\mathbf{x}^t\}$ s.t.

$$f(\mathbf{x}^{t+1}) < f(\mathbf{x}^t), \quad t = 0, 1, \ldots$$

Iterative descent algorithms

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- $\mathbf{d}$ is said to be a **descent direction** of f at $\mathbf{x}$ if

$$\underbrace{f'(\mathbf{x}; \mathbf{d}) := \lim_{\tau \downarrow 0} \frac{f(\mathbf{x} + \tau \mathbf{d}) - f(\mathbf{x})}{\tau}}_{\text{directional derivative}} = \nabla f(\mathbf{x})^\top \mathbf{d} < 0 \tag{1}$$

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In each iteration, search minimum in a descent direction

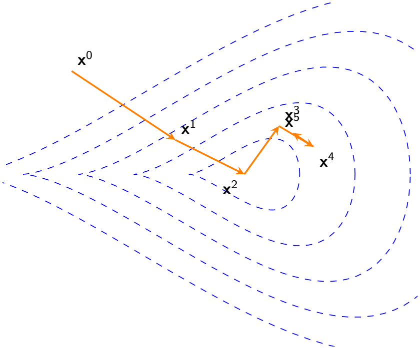
$$\mathbf{x}^{t+1} = \mathbf{x}^t + \eta_t \mathbf{d}^t \tag{2}$$

where $\mathbf{d}^t$: descent direction at $\mathbf{x}^t$; $\eta_t > 0$: stepsize

Gradient descent (GD)

One of the most important examples of (2): **gradient descent**

$$\mathbf{x}^{t+1} = \mathbf{x}^{t} - \eta_t \nabla f(\mathbf{x}^{t}) \tag{3}$$



- traced to Augustin Louis Cauchy '1847 ...

Gradient descent (GD) - steepest descent

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$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta_t \nabla f(\mathbf{x}^t) \tag{3}$$

- descent direction: $\mathbf{d}^t = -\nabla f(\mathbf{x}^t)$
- a.k.a. **steepest descent**, since from (1) and Cauchy-Schwarz (CS),

$$\underbrace{\arg \min_{\mathbf{d}:||\mathbf{d}||_2 \leq 1} f'(\mathbf{x};\mathbf{d}) = \arg \min_{\mathbf{d}:||\mathbf{d}||_2 \leq 1} \nabla f(\mathbf{x})^\top \mathbf{d} = -\frac{\nabla f(\mathbf{x})}{||\nabla f(\mathbf{x})||_2}}_{\text{direction with the greatest rate of objective value improvement}}$$

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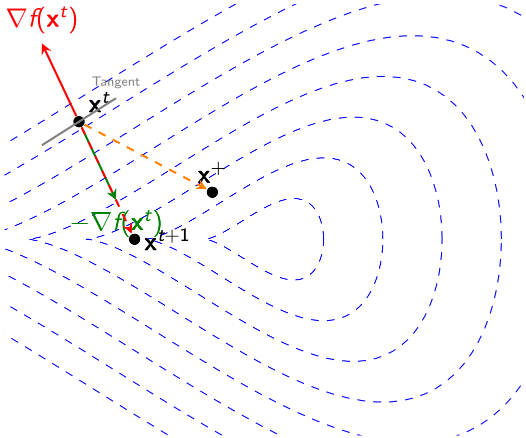
The **CS inequality** gives us a lower bound $\mathbf{u}^\top \mathbf{v} \ge -\|\mathbf{u}\|_2\|\mathbf{v}\|_2$, which is achieved when $\mathbf{v} = -c \cdot \mathbf{u}$ for some scalar $c > 0$.

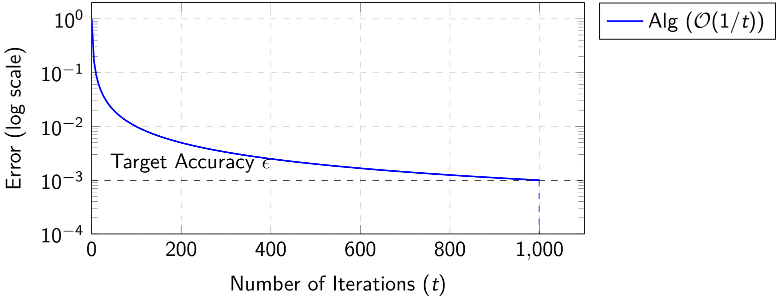
Gradient descent (GD) - steepest descent



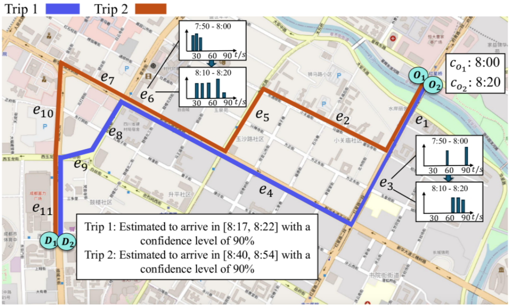
Gradient descent is great. But when it will terminate?

In the real world, we have a limited budget. How many iterations are needed to reach a good-enough solution?

Convergence analysis gives us the answer. It tells us how an algorithm will perform at scale.



Convergence analysis as means to obtain ETA



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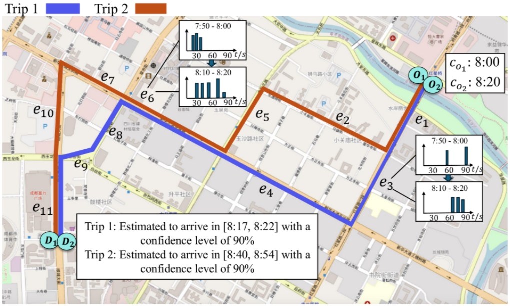

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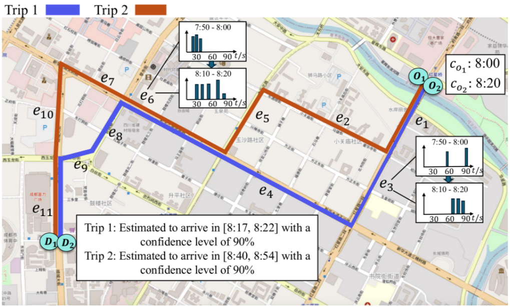

- How many miles I can drive per hour given the total distance?
- How much progress I make per hour given the remaining distance?

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Quadratic minimization

To get a sense of the convergence rate of GD, let's begin with quadratic objective functions (e.g., in linear regression)

$$\min_{\mathbf{x}} \; f(\mathbf{x}) := \frac{1}{2}(\mathbf{x} - \mathbf{x}^*)^\top \mathbf{Q}(\mathbf{x} - \mathbf{x}^*)$$

for some $n \times n$ matrix $\mathbf{Q} \succ 0$, where $\nabla f(\mathbf{x}) = \mathbf{Q}(\mathbf{x} - \mathbf{x}^*)$

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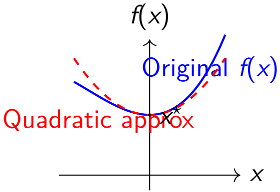
Accordingly, the GD update rule becomes

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta_t \nabla f(\mathbf{x}^t) = (\mathbf{I} - \eta_t \mathbf{Q})(\mathbf{x}^t - \mathbf{x}^*) + \mathbf{x}^*!$$

What is unique about quadratic minimization?

Quadratic minimization

- **Local approximation:** Any general smooth function behaves like a quadratic very close to a minimizer (according to Taylor's theorem).



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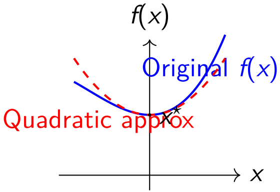

- **Tractable analysis:** Allow to derive exact, closed-form convergence rates. The insights we gain apply to more complex problems.

$$\boxed{\mathbf{x}^t - \mathbf{x}^* = \left(\prod_{k=0}^{t-1}(\mathbf{I} - \eta_k \mathbf{Q})\right)(\mathbf{x}^0 - \mathbf{x}^*)}.$$

Convergence for constant stepsizes

Proof: According to the GD update rule,

$$\mathbf{x}^{t+1} - \mathbf{x}^* = \mathbf{x}^t - \mathbf{x}^* - \eta_t \nabla f(\mathbf{x}^t) = (\mathbf{I} - \eta_t \mathbf{Q})(\mathbf{x}^t - \mathbf{x}^*)$$
$$\implies ||\mathbf{x}^{t+1} - \mathbf{x}^*||_2 \leq ||\mathbf{I} - \eta_t \mathbf{Q}|| \cdot ||\mathbf{x}^t - \mathbf{x}^*||_2$$

To get the fastest convergence, we must choose the stepsize η that **minimizes the contraction factor** $||\mathbf{I} - \eta \mathbf{Q}||_2$.

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$$\Longrightarrow \; \|\mathbf{x}^{t+1} - \mathbf{x}^*\|_2 \leq \|\mathbf{I} - \eta_t \mathbf{Q}\| \cdot \|\mathbf{x}^t - \mathbf{x}^*\|_2$$

To get the fastest convergence, we must choose the stepsize η that **minimizes the contraction factor** $\|\mathbf{I} - \eta \mathbf{Q}\|_2$.

$$\|\mathbf{I} - \eta \mathbf{Q}\| = \underbrace{\max\{|1 - \eta\lambda_1(\mathbf{Q})|, |1 - \eta\lambda_n(\mathbf{Q})|\}}_{\text{remark: optimal choice is } \eta_t = \frac{2}{\lambda_1(\mathbf{Q}) + \lambda_n(\mathbf{Q})}}$$
$$= 1 - \frac{2\lambda_n(\mathbf{Q})}{\lambda_1(\mathbf{Q}) + \lambda_n(\mathbf{Q})} = \frac{\lambda_1(\mathbf{Q}) - \lambda_n(\mathbf{Q})}{\lambda_1(\mathbf{Q}) + \lambda_n(\mathbf{Q})}$$

Apply the above bound recursively to complete the proof. $\square$

Convergence for constant stepsizes

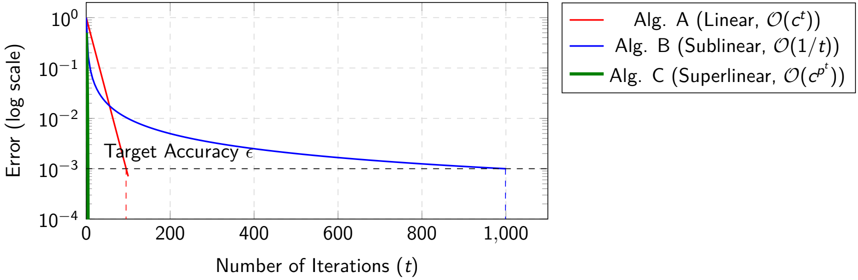
Convergence rate: if $\eta_t \equiv \eta = \frac{2}{\lambda_1(\mathbf{Q})+\lambda_n(\mathbf{Q})}$, then

$$\|\mathbf{x}^t - \mathbf{x}^*\|_2 \le \left(\frac{\lambda_1(\mathbf{Q}) - \lambda_n(\mathbf{Q})}{\lambda_1(\mathbf{Q}) + \lambda_n(\mathbf{Q})}\right)^t \|\mathbf{x}^0 - \mathbf{x}^*\|_2$$

where $\lambda_1(\mathbf{Q})$ (resp. $\lambda_n(\mathbf{Q})$) is the largest (smallest) eigenvalue of $\mathbf{Q}$.

- often called **linear convergence** or **geometric convergence**
- since the error lies below a log-linear plot of error vs. iteration count

Different rates of convergence speed



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where $\lambda_1(\mathbf{Q})$ (resp. $\lambda_n(\mathbf{Q})$) is the largest (smallest) eigenvalue of $\mathbf{Q}$.

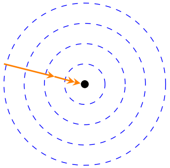
- the convergence rate is dictated by the **condition number**

$$\kappa := \frac{\lambda_1(\mathbf{Q})}{\lambda_n(\mathbf{Q})} \text{ of } \mathbf{Q}\text{, or equivalently, } \kappa := \frac{\max_{\mathbf{x}} \lambda_1(\nabla^2 f(\mathbf{x}))}{\min_{\mathbf{x}} \lambda_n(\nabla^2 f(\mathbf{x}))}$$

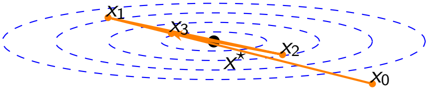
The impact of the condition number κ

The condition number of $\mathbf{Q}$ dictates the geometry of the loss surface.

Well-conditioned ($\kappa \approx 1$)



Ill-conditioned ($\kappa \gg 1$)



$\Rightarrow$ When contours are circular, the negative gradient points directly at the minimum. Convergence is fast.

$\Rightarrow$ When contours are highly elliptical, the gradient is almost orthogonal to the direction of the minimum, causing zig-zags.

Exact line search

The stepsize rule $\eta_t \equiv \eta = \frac{2}{\lambda_1(\mathbf{Q})+\lambda_n(\mathbf{Q})}$ relies on the spectrum of $\mathbf{Q}$, which requires preliminary experimentation.

Another more practical strategy is the **exact line search** rule

$$\eta_t = \arg\min_{\eta \geq 0} f(\mathbf{x}^t - \eta \nabla f(\mathbf{x}^t)) \tag{4}$$

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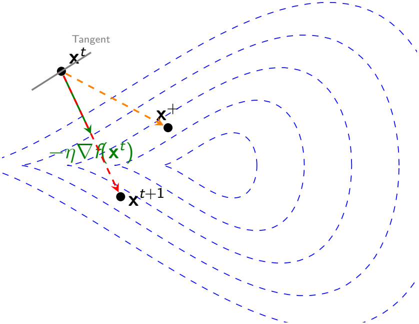

Convergence for exact line search*

Convergence rate: if $\eta_t = \arg\min_{\eta \geq 0} f(\mathbf{x}^t - \eta \nabla f(\mathbf{x}^t))$, then

$$f(\mathbf{x}^t) - f(\mathbf{x}^*) \leq \left(\frac{\lambda_1(\mathbf{Q}) - \lambda_n(\mathbf{Q})}{\lambda_1(\mathbf{Q}) + \lambda_n(\mathbf{Q})} \right)^{2t} \left(f(\mathbf{x}^0) - f(\mathbf{x}^*) \right)$$

- stated in terms of the objective values
- convergence rate not faster than the constant stepsize rule

Convergence for exact line search*

Proof: For notational simplicity, let $\mathbf{g}^t = \nabla f(\mathbf{x}^t) = \mathbf{Q}(\mathbf{x}^t - \mathbf{x}^*)$. It can be verified that exact line search gives (only holds for quadratic loss)

$$\eta_t = \frac{(\mathbf{g}^t)^\top \mathbf{g}^t}{(\mathbf{g}^t)^\top \mathbf{Q}\mathbf{g}^t}.$$

Using $f(\mathbf{x}^t) = \frac{1}{2}(\mathbf{x}^t - \mathbf{x}^*)^\top \mathbf{Q}(\mathbf{x}^t - \mathbf{x}^*) = \frac{1}{2}(\mathbf{g}^t)^\top \mathbf{Q}^{-1}\mathbf{g}^t$, this gives

$$\begin{aligned}
f(\mathbf{x}^{t+1}) &= \frac{1}{2}(\mathbf{x}^t - \eta_t \mathbf{g}^t - \mathbf{x}^*)^\top \mathbf{Q}(\mathbf{x}^t - \eta_t \mathbf{g}^t - \mathbf{x}^*) \\
&= \frac{1}{2}(\mathbf{x}^t - \mathbf{x}^*)^\top \mathbf{Q}(\mathbf{x}^t - \mathbf{x}^*) - \eta_t ||\mathbf{g}^t||_2^2 + \frac{\eta_t^2}{2}(\mathbf{g}^t)^\top \mathbf{Q}\mathbf{g}^t \\
&= \frac{1}{2}(\mathbf{x}^t - \mathbf{x}^*)^\top \mathbf{Q}(\mathbf{x}^t - \mathbf{x}^*) - \frac{||\mathbf{g}^t||_2^4}{2(\mathbf{g}^t)^\top \mathbf{Q}\mathbf{g}^t} \\
&= \left(1 - \frac{||\mathbf{g}^t||_2^4}{((\mathbf{g}^t)^\top \mathbf{Q}\mathbf{g}^t)(((\mathbf{g}^t)^\top \mathbf{Q}^{-1}\mathbf{g}^t)}\right) f(\mathbf{x}^t).
\end{aligned}$$

Convergence for exact line search*

Proof (cont.): From Kantorovich's inequality

$$\frac{||\mathbf{y}||_2^4}{(\mathbf{y}^\top \mathbf{Q}\mathbf{y})(\mathbf{y}^\top \mathbf{Q}^{-1}\mathbf{y})} \geq \frac{4\lambda_1(\mathbf{Q})\lambda_n(\mathbf{Q})}{(\lambda_1(\mathbf{Q})+\lambda_n(\mathbf{Q}))^2},$$

we arrive at

$$\begin{aligned} f(\mathbf{x}^{t+1}) &\leq \left(1 - \frac{4\lambda_1(\mathbf{Q})\lambda_n(\mathbf{Q})}{(\lambda_1(\mathbf{Q})+\lambda_n(\mathbf{Q}))^2}\right) f(\mathbf{x}^t) \\ &= \left(\frac{\lambda_1(\mathbf{Q})-\lambda_n(\mathbf{Q})}{\lambda_1(\mathbf{Q})+\lambda_n(\mathbf{Q})}\right)^2 f(\mathbf{x}^t) \end{aligned}$$

This concludes the proof since $f(\mathbf{x}^*) = \min_{\mathbf{x}} f(\mathbf{x}) = 0$ $\square$

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In-Class Lab: Calculating the descent

Goal: To manually compute the first few steps of Gradient Descent and see how the learning rate (η) affects convergence.

The Setup

- **Our function:** A simple parabola, $f(x) = x^2$.
- **Its gradient:** $f'(x) = 2x$. The minimum is at $x = 0$.
- **The GD update rule:** $x_{t+1} = x_t - \eta \cdot f'(x_t)$.

Part 1: A "Good" learning rate

Let's start at $\mathbf{x_0} = \mathbf{4}$ with a learning rate of $\eta = \mathbf{0.1}$.

Instructions: Fill out the table below for the first 3 steps of GD.

$\mathbf{t}$	$\mathbf{x_t}$	$\mathbf{f'(x_t) = 2x_t}$	$\eta \cdot \mathbf{f'(x_t)}$	$\mathbf{x_{t+1}}$
0	4	8	0.8	3.2
1	3.2			
2				

Question

What do you observe about the value of x_t? Is it approaching the minimum at $x = 0$?

Part 2: A “Bad” learning rate

Let's see what happens if the learning rate is too large. Start again at $\mathbf{x_0} = \mathbf{4}$ but with $\eta = \mathbf{1.1}$.

Instructions: Fill out the table for the first 3 steps.

$\mathbf{t}$	$\mathbf{x_t}$	$\mathbf{f'(x_t) = 2x_t}$	$\eta \cdot \mathbf{f'(x_t)}$	$\mathbf{x_{t+1}}$
0	4	8	8.8	-4.8
1	-4.8			
2				

Question

What is happening to the value of x_t now? Is the algorithm converging?

Part 3: Backtracking line search

Instead of a fixed η, let's find one automatically at the first step ($t = 0$).

- Start at $\mathbf{x_0} = \mathbf{4}$ and backtracking parameters: $\alpha = \mathbf{0.5}$, $\beta = \mathbf{0.5}$.
- Start with an initial guess of $\eta = \mathbf{1.0}$.

Instructions: Check the Armijo condition. If it's true, update $\eta \leftarrow \beta\eta$ and check again. Stop when the condition is false.

$$\textbf{Check if}: \quad f(x_t - \eta \nabla f(x_t)) > f(x_t) - \alpha\eta ||\nabla f(x_t)||_2^2$$

Current η	**LHS**: $f(4 - \eta \cdot 8)$	**RHS**: $16 - 0.5 \cdot \eta \cdot 64$	**Is LHS > RHS?**
1.0	$(4-8)^2 = 16$	$16 - 32 = -16$	Yes
0.5			
...			

What is the final step size η_0 accepted by the algorithm? Using this η_0, what is the next point, x_1?

Solutions: The effect of the learning rate

Part 1: Converging ($\eta = 0.1$)

$\mathbf{t}$	$\mathbf{x_t}$	$\mathbf{f'(x_t)}$	$\eta \cdot \mathbf{f'(x_t)}$	$\mathbf{x_{t+1}}$
0	4.0	8.0	0.8	3.2
1	3.2	6.4	0.64	2.56
2	2.56	5.12	0.512	2.048

Part 2: Diverging ($\eta = 1.1$)

$\mathbf{t}$	$\mathbf{x_t}$	$\mathbf{f'(x_t)}$	$\eta \cdot \mathbf{f'(x_t)}$	$\mathbf{x_{t+1}}$
0	4.0	8.0	8.8	-4.8
1	-4.8	-9.6	-10.56	5.76
2	5.76	11.52	12.672	-6.912

A learning rate that is too large can cause the algorithm to overshoot the minimum and diverge completely.

Part 3: Backtracking solution: The final accepted step size is $\eta_0 = \mathbf{0.5}$. The next point is:

$$x_1 = x_0 - \eta_0 \cdot f'(x_0) = 4 - 0.5 \cdot 8 = 0$$

Backtracking prevents divergence by finding a safe stepsize automatically.

Recap and fine-tuning

- What we have talked about today?
  - $\Rightarrow$ What is gradient descent and why it works?
  - $\Rightarrow$ What is its performance on quadractic minimization?

Welcome anonymous survey!