Statistical (Machine) Learning

Lecture 10 — Optimization basics

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Optimization for ML

Act 1 of 2: Uncontrained Optimization

Optimization basics

- The function we're trying to optimize is the **objective function** generically denoted by $M(\cdot)$
- The argument to $M(\cdot)$ is θ
  - Some people call this the **optimand**
- The possible values of θ is Θ, the **domain** or **feasible set**, whose dimension is p
- **Optimization** can be minimization or maximization, as we like; we'll stick with *minimizing*

Local vs Global minima

- θ is a **global minimum** when

$$\theta' \neq \theta \quad \Rightarrow \quad M(\theta') \geqslant M(\theta) \quad \text{not necessarily unique!}$$

- θ is a **local minimum** when $M(\theta) \leqslant M(\theta')$ whenever θ' is *close enough* to θ
  - Every global minimum is also a local minimum
  - If there's only one local minimum anywhere, it's the global minimum
- Lots of local minima tend to make it harder to find the global minimum

At "the" minimum: value vs location

- If $\theta^\star$ is a global minimum, then $M(\theta^\star)$ is the **value** of the minimum or minimal value, in symbols

$$\min_{\theta \in \Theta} M(\theta)$$

- But $\theta^\star$ itself is the **location** of the global minimum, in symbols

$$\operatorname{argmin}_{\theta \in \Theta} M(\theta)$$

- **Example**: the minimal value of $(x-1)^2$ is 0, but the location of the minimum is $x = 1$
- Both value and location can change with $\Theta \rightsquigarrow$ important when we look at **constraints** later

Finding the minimum: optimization algorithms

- An optimization algorithm starts from M and Θ, and possibly an initial guess $\theta^{(0)}$, and returns an **approximation** to $\operatorname{argmin}_{\theta \in \Theta} M(\theta)$, call it θ_{out}
- We usually measure the approximation by difference in the *value*, not the location: the algorithm gets ϵ-close when

$$M(\theta_{\text{out}}) \leqslant \epsilon + \min_{\theta \in \Theta} M(\theta)$$

- Often, the longer we let the algorithm run, the better the approximation
  - How many steps does the algorithm need to get ϵ-close to the optium?
    $O(1/\epsilon)$ or $O(\epsilon^{-d})$ would be polynomial, $O(\log 1/\epsilon)$ would be logarithmic, $\mathrm{e}^{O(1/\epsilon)}$ would be exponential (and bad!)
- Going forward, **early stopping** (an optimization algorithm) will be one of many ways to *regularize* our learning algorithms to avoid **overfitting**.

So how do we build an optimization algorithm anyway?

- Start with *calculus*, assume $M(\cdot)$ has as many derivatives with respect to θ as we need
- **1st-order condition**: at an (interior!) local minimum/maximum, or inflection point,

$$\nabla M(\theta) = 0 \quad \rightsquigarrow \quad M \text{ is flat at the minimum}$$

- **2nd-order condition**: at an (interior) local *minimum* only, for any direction $\boldsymbol{v} \neq 0$,

$$\boldsymbol{v} \left(\nabla \nabla M(\theta) \right) \boldsymbol{v} \geqslant 0 \quad (\text{strictly positive in at least some directions})$$

  - $\nabla \nabla M$ is the matrix of 2nd partial derivatives, or **Hessian**, so I will also write $\mathbf{h}(\theta)$
  - This condition is what's meant when we say the Hessian is **non-negative-definite**: $\mathbf{h}(\theta) \succeq 0$
  - **Positive-definite**: $\mathbf{h}(\theta) \succ 0$, means $\boldsymbol{v}\,\mathbf{h}\,\boldsymbol{v} > 0$ for all $\boldsymbol{v} \neq 0$; this implies θ is an *isolated* local minimum
  - **In words**: moving away from the local minimum in any direction can only increase the objective function

Optimizing by equation-solving

- One approach: use the first-order condition to get a system of equations

$$\nabla M(\theta) = 0$$

  - We have one equation per coordinate of θ
  - When M is empirical risk $\widehat{R}$, sometimes called the **estimating equations** or even **normal equations**
- Solve the system of equations for θ
- If there's more than one solution, check the second-order conditions
- This is what we did for estimating linear models by ordinary least squares, or even weighted least squares

Pros and cons of the solve-the-equations approach

- You need to *set up* the system of equations, and often finding ∇M would itself be a pain
  - However, **numerical differentiation** is quite widespread nowaday
- You need to solve a system of equations: good if there are good **solvers** for that type of system of equations, not so good otherwise
  - For **linear systems**, even very old-fashioned methods that go back to Gauss get ϵ approximations with $O(\log 1/\epsilon)$ iterations
  - General-purpose **nonlinear** equation-solving is still much *harder*
    - sometimes works by using Taylor expansion to linearize
    - sometimes works by turning the solve-the-equations into "*minimize the difference between the left and the right hand side of the equation*"

Computer differentiation: a few words (Nocedal and Wright, 2006)

1. Use a **computer algebra system**, such as Mathematica/Wolfram Alpha or Maxima.
   - Works well for relatively simple models $\rightsquigarrow$ the results quite often require "hand simplification"
2. Approximate derivative using **finite difference** $\rightsquigarrow$ always possible but less accurate than other methods

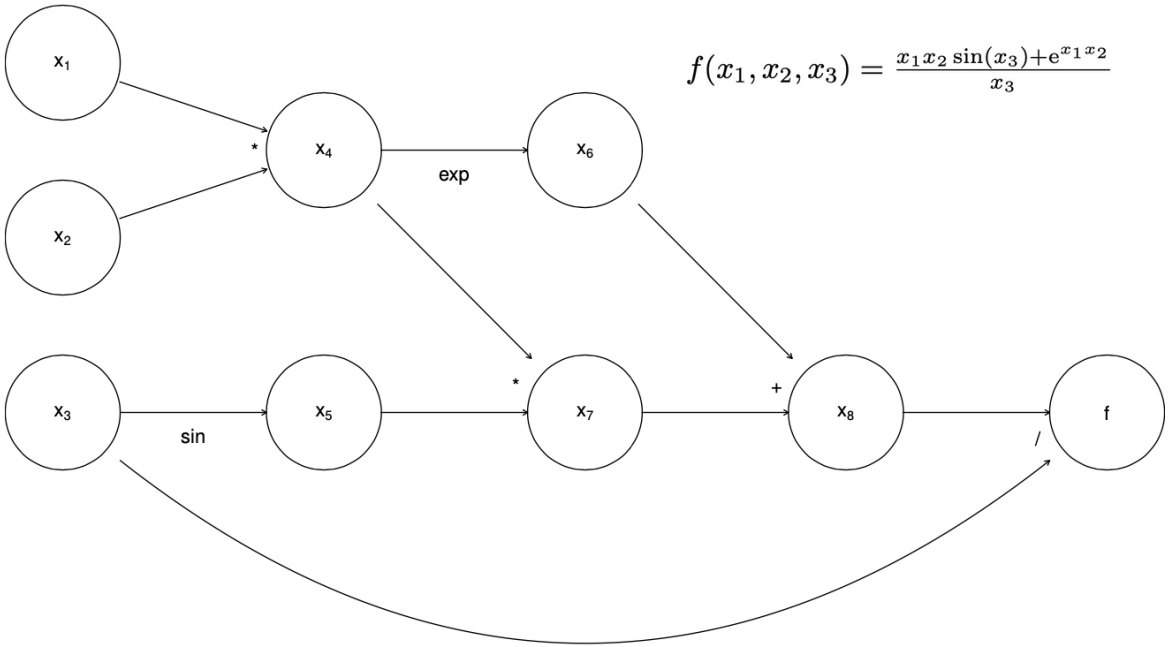
$$\frac{\partial M}{\partial \theta_j} \approx \frac{M(\boldsymbol{\theta} + \Delta \boldsymbol{e}_j) - M(\boldsymbol{\theta})}{\Delta} \quad \texttt{forward differencing}$$

$$\frac{\partial M}{\partial \theta_j} \approx \frac{M(\boldsymbol{\theta} + \Delta \boldsymbol{e}_j) - M(\boldsymbol{\theta} - \Delta \boldsymbol{e}_i)}{2\,\Delta} \quad \texttt{centred differencing}$$

   - *Centred differencing* is typically more accurate but also more costly than *forward differencing*.
   - *Higher order* derivatives can also be approximated similarly.
   - How big should Δ be? As *small* as possible? **Nope**! Because of your computer *finite precision*, to avoid *cancellation error* you have to trade-off!
3. Use **automatic differentiation** (AD), which computes numerically **exact** derivative directly from the code implementing the function to be differentiated, by automatic application of the **chain rule**.
   - As with *finite difference*, there are two main AD *modes*: a *forward*-mode and a *reverse*-mode. The latter comes with the potential for *big* computational savings but *heavy* storage requirements because of the "direction" of the derivative propagation.

Computer differentiation: a few words (Nocedal and Wright, 2006)

- To better understand what I mean by "*direction of the derivative propagation*", we need to introduce the concept of **computational graph** that details how your computer breaks down the computation into a sequence of elementary operations.



  - The nodes x_4 and x_8 are intermediate quantities to get to the final answer.
  - The arrows run from *parent* to *child* nodes: **no** child can be evaluated before any of its parents.

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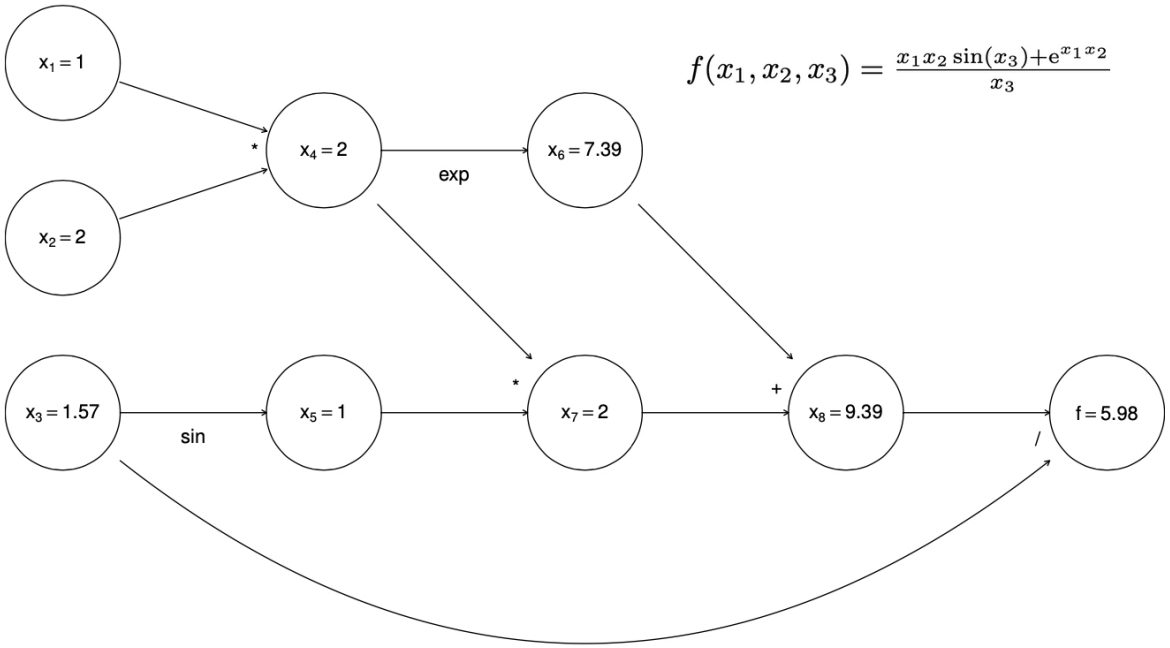

  - The arrows run from *parent* to *child* nodes: **no** child can be evaluated before any of its parents.
  - An example of simple *left-to-right* evaluation

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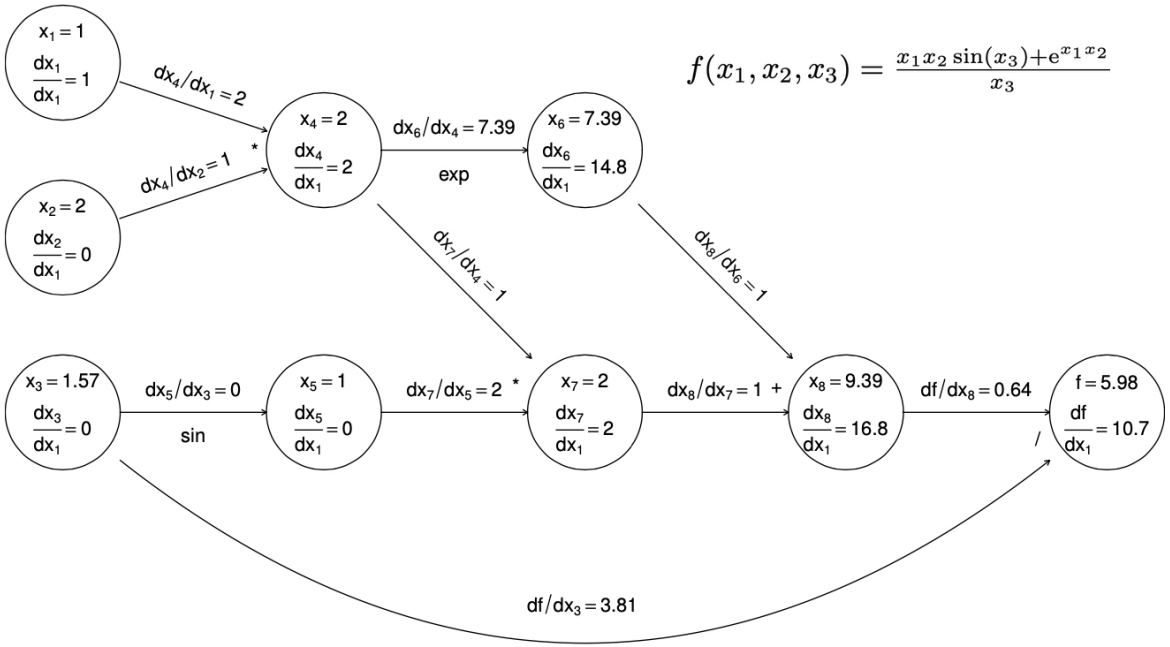

  - *Forward-mode* carries derivatives forward through the graph alongside values.
  - For example, the derivative of a node w.r.t. x_1 is computed using: $\frac{\partial x_k}{\partial x_1} = \sum_{\{j \text{ parent of } k\}} \frac{\partial x_k}{\partial x_j} \frac{\partial x_j}{\partial x_1}$

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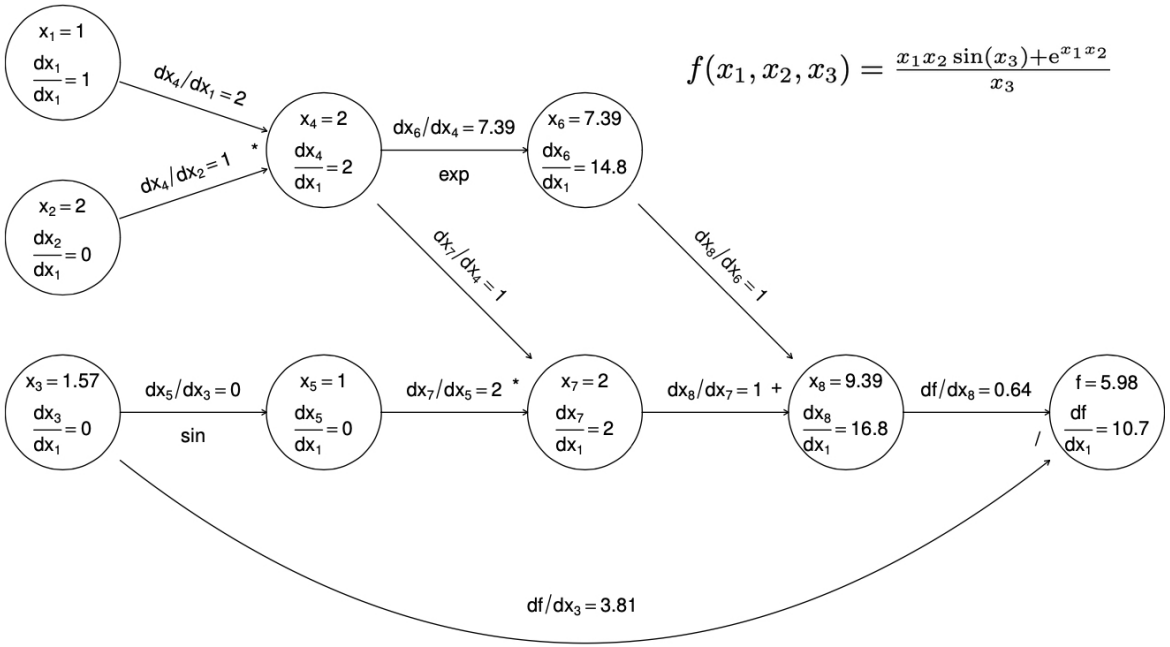

  - **Pro**: we could discard the values and derivatives of a node *as soon as* all its children are evaluated
  - **Con**: if many derivatives are required, the theoretical computational cost is similar to finite difference (as many operations are required for *each* derivative as are required for function evaluation)

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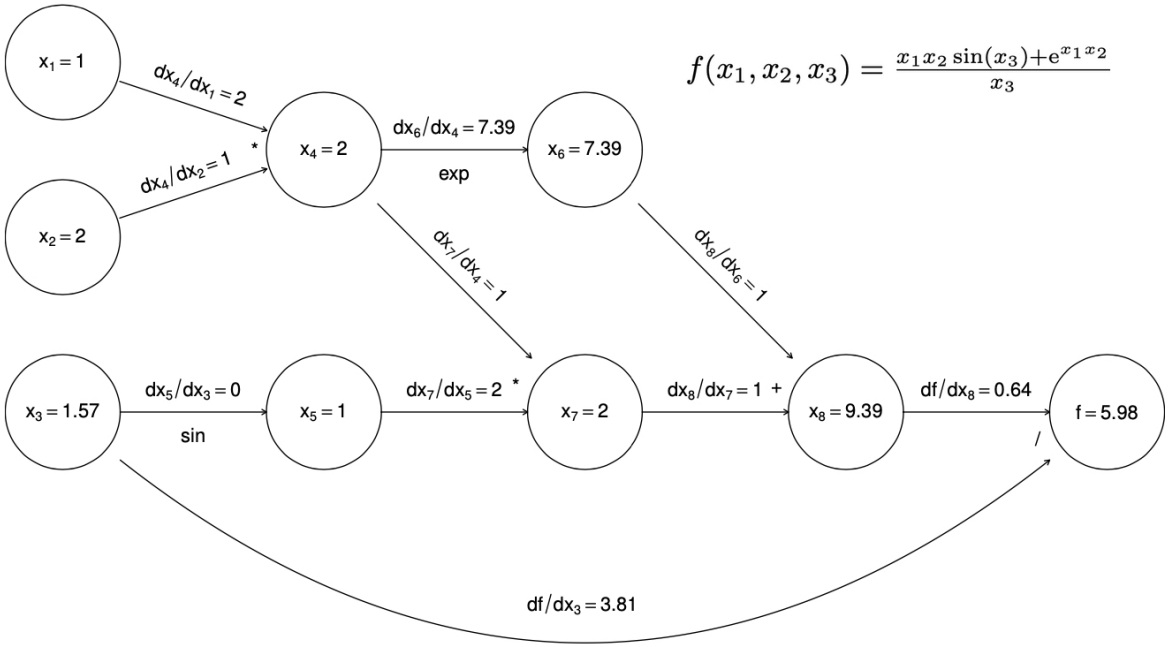

  - *Reverse-mode* first executed a *forward sweep* evaluating the function and all the derivatives of nodes w.r.t. parents.

Computer differentiation: a few words (Nocedal and Wright, 2006)

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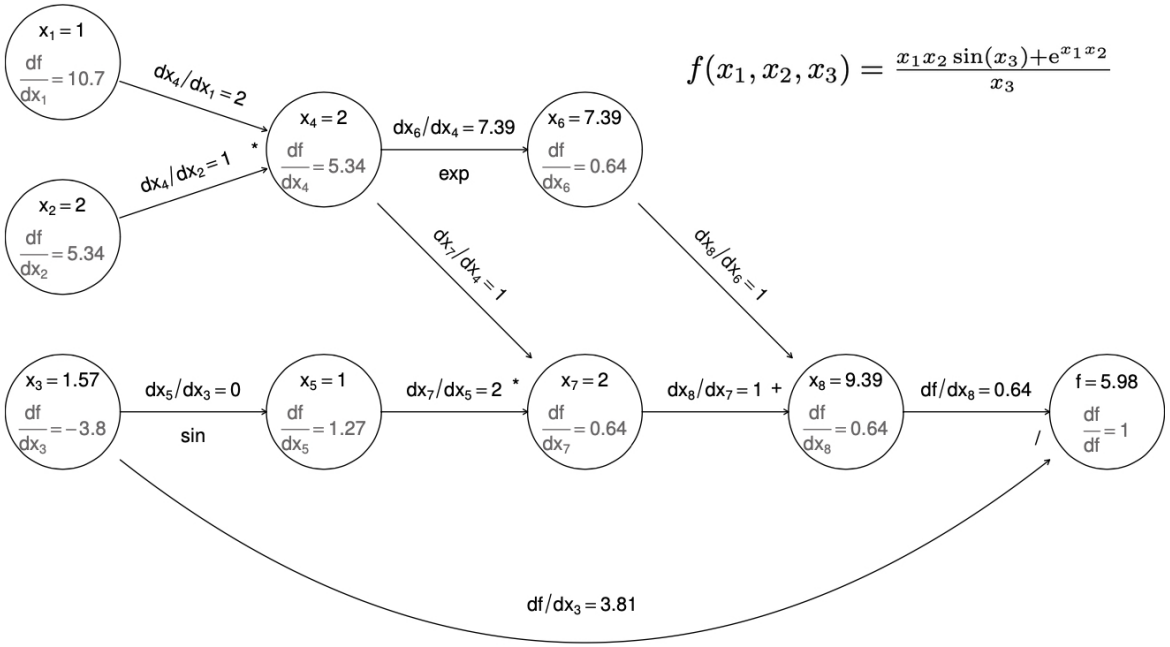

  - *Reverse-mode* then executed a *reverse sweep* that works backward from the terminal node, where $\partial f / \partial f = 1$, evaluating the derivative of f w.r.t. each node (in gray) using: $\frac{\partial f}{\partial x_k} = \sum_{\{j \text{ is child of } k\}} \frac{\partial x_j}{\partial x_k} \frac{\partial f}{\partial x_j}$

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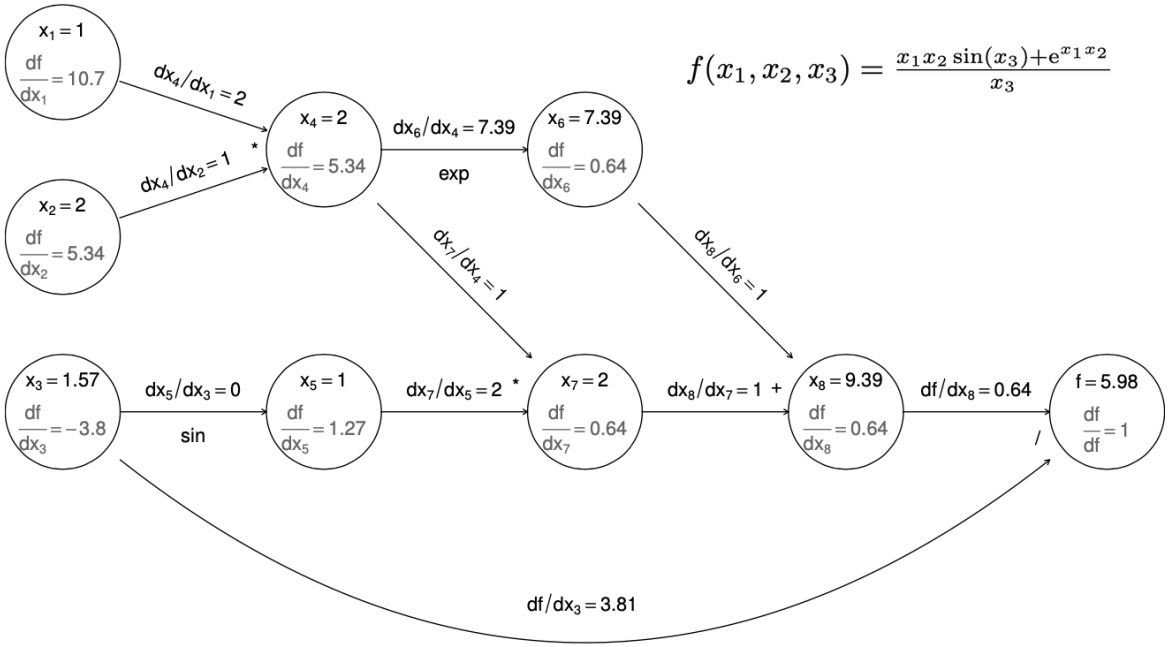


  - **Pro**: now there is only one derivative to be evaluated at each node, but in the end we know the derivative of f w.r.t. every input variable.
  - **Con**: The values of *all nodes* and the evaluated derivatives associated with *every connection* have to be stored during the *forward sweep* in order to be used in the *reverse sweep*.

Computer differentiation: a few packages

$$M(a, x) = \frac{1}{x^2 \sin(a\ x)}$$

```
dx <- D( expression( 1/( x^2*sin(a*x)) ), "x"); dx
```

```
-((2 * x * sin(a * x) + x^2 * (cos(a * x) * a))/(x^2 * sin(a *
    x))^2)
```

$$M(x_1, x_2, x_3) = \frac{x_1 x_2 \sin(x_3) + e^{x_1 x_2}}{x_3}$$

```
# For not overly complex function, we may try <deriv>
M  <- expression( (x1*x2*sin(x3) + exp(x1*x2))/x3)
gr <- deriv(M, c("x1", "x2", "x3"), function.arg = c("x1", "x2", "x3"))
gr(1, 2, pi/2)
```

```
[1] 5.977259
attr(,"gradient")
           x1       x2        x3
[1,] 10.68128 5.340639 -3.805241
```

Go back to the calculus

Gradient Descent

1. Start with a guess $\theta^{(0)}$
2. Find $\nabla M(\theta^{(0)})$
3. Move in the **opposite** direction:

$$\theta^{(1)} = \theta^{(0)} - a_0 \nabla M(\theta^{(0)})$$

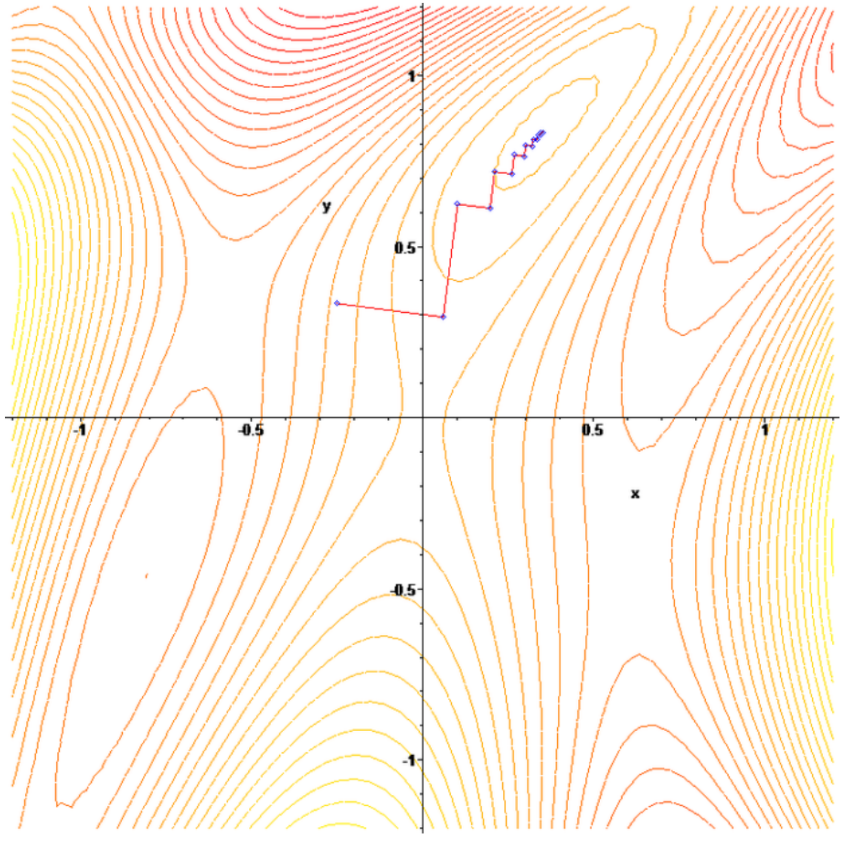
4. Repeat:

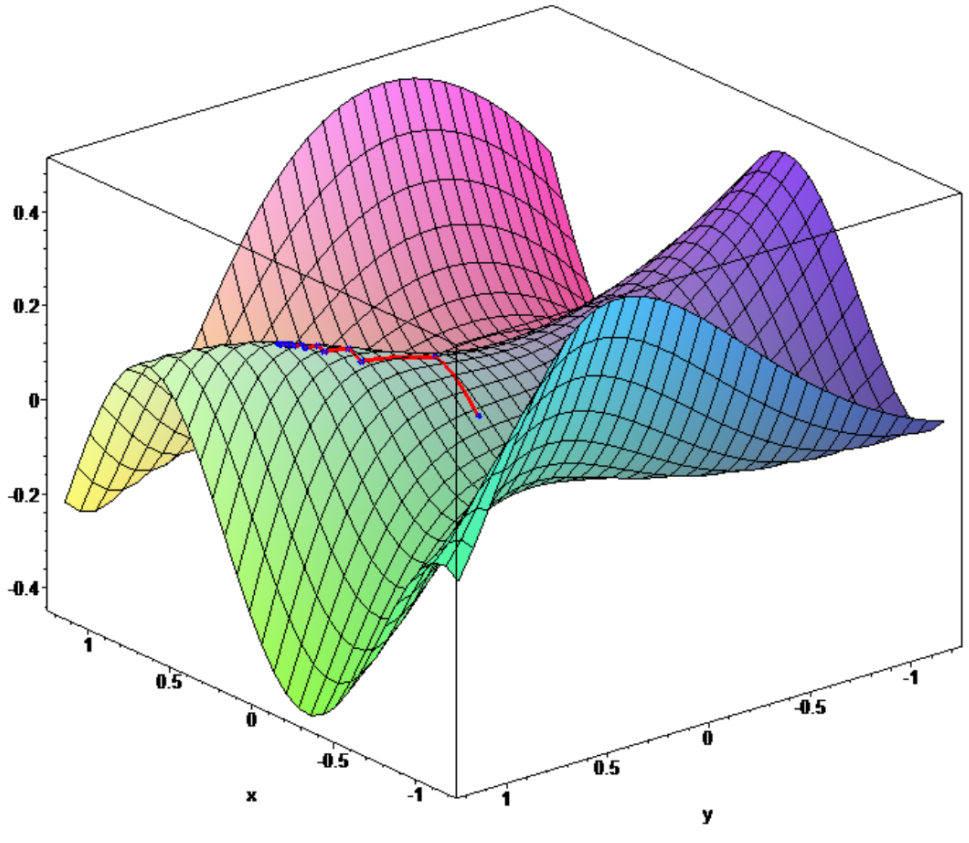
$$\theta^{(t+1)} = \theta^{(t)} - a_t \nabla M(\theta^{(t)})$$

- **Remark**: a *local* optimum will be a **fixed point**
- **Issue**: how big are the **step sizes** (a.k.a. *learning rate*) a_t?

Go back to the calculus

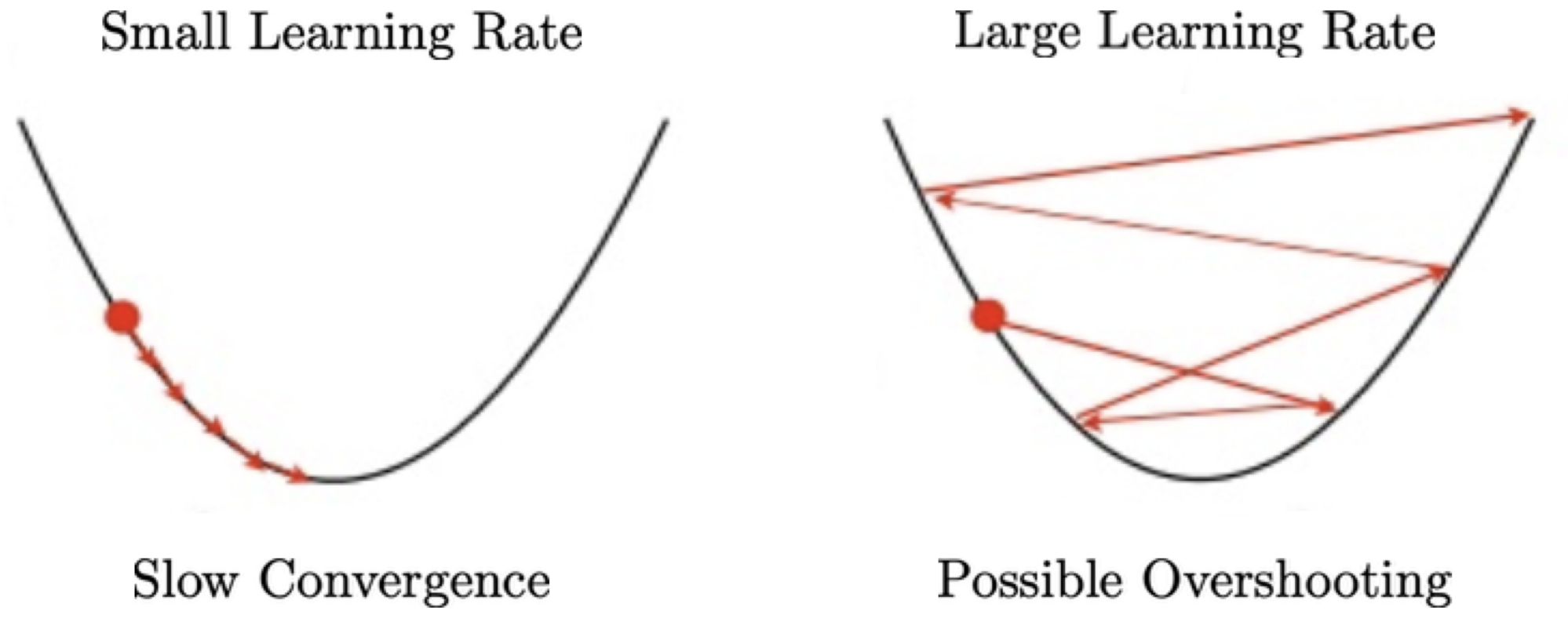
Gradient Descent





Go back to the calculus

Gradient Descent



Constant-step-size gradient descent

- **Inputs**: objective function M, step size a, initial guess $\theta^{(0)}$
- **While**: (*not too tired*) and (*making adequate progress*)
  - **Find**: $\nabla M(\theta^{(t)})$
  - **Set**: $\theta^{(t+1)} \leftarrow \theta^{(t)} - a\nabla M(\theta^{(t)})$
- Return final θ

- "*not too tired*" = $\{$set a maximum number of iterations$\}$
- "*making adequate progress*" = $\{M$ isn't changing by too little$\}$ and/or $\{\theta$ isn't changing by too little$\}$ and/or $\{\nabla M$ isn't too close to zero$\}$

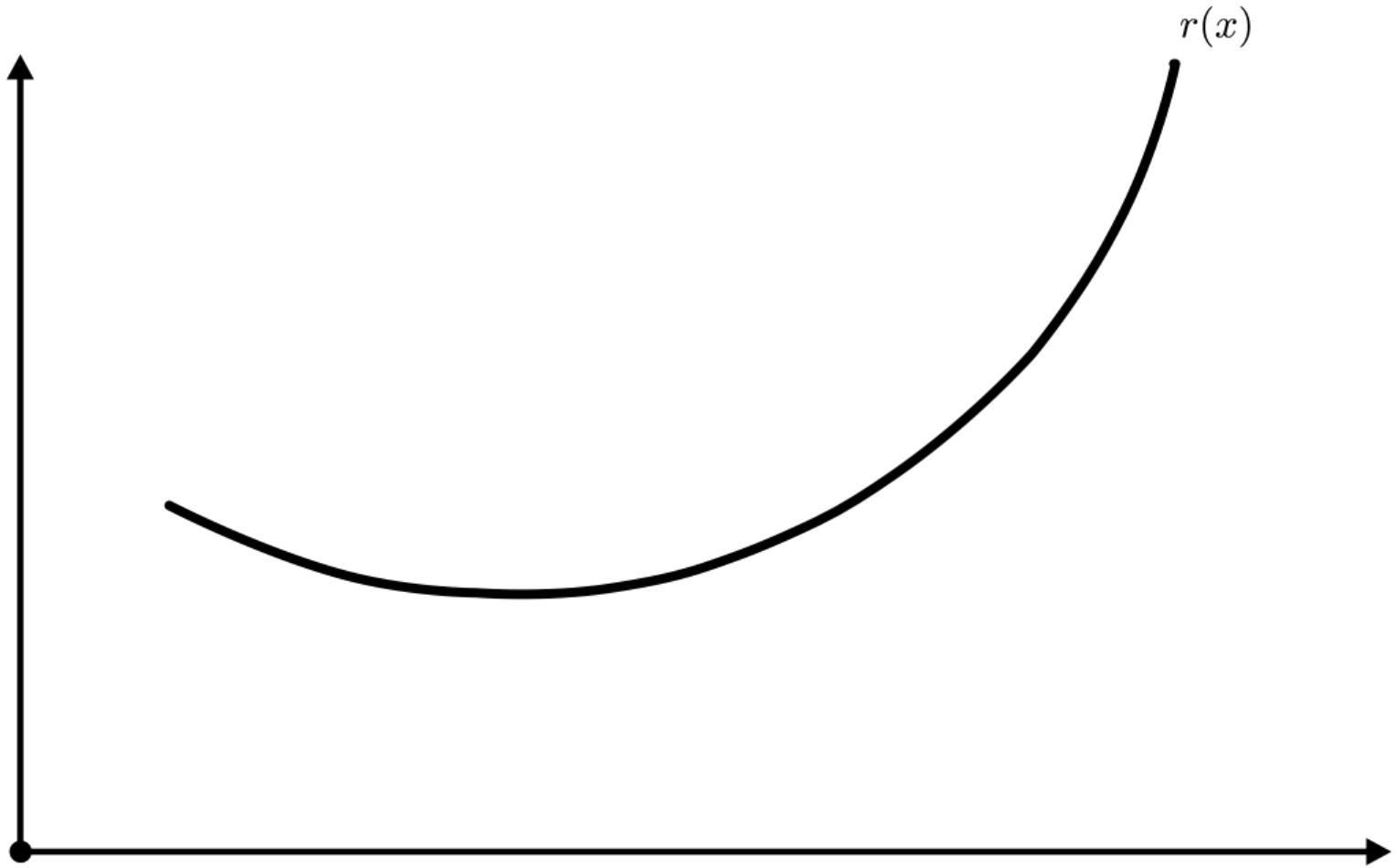
Constant-step-size gradient descent

- Pick an $a > 0$ that's small and use it at each step
- Each iteration of gradient descent takes $O(p)$ operations
    - Find p derivatives, multiply by a, add to $\theta^{(t-1)}$

Constant-step-size gradient descent

- Pick an $a > 0$ that's small and use it at each step
- Each iteration of gradient descent takes $O(p)$ operations
  - Find p derivatives, multiply by a, add to $\theta^{(t-1)}$
- **IF** M is *nice*, $\theta^{(t)}$ is an ϵ-approximation of the optimum after $t = O(\epsilon^{-2})$ iterations
  - In other words, at that point $M(\theta^{(t)}) \leqslant \epsilon + \min M(\theta)$
  - "*Nice*" here means: **convex** and *second-differentiable*
- **IF** M is **very** *nice*, $\theta^{(t)}$ is an ϵ-approximation after only $t = O(\log 1/\epsilon)$ iterations
  - "*Nice*" + **strictly** convex

Convexity is and will be crucial



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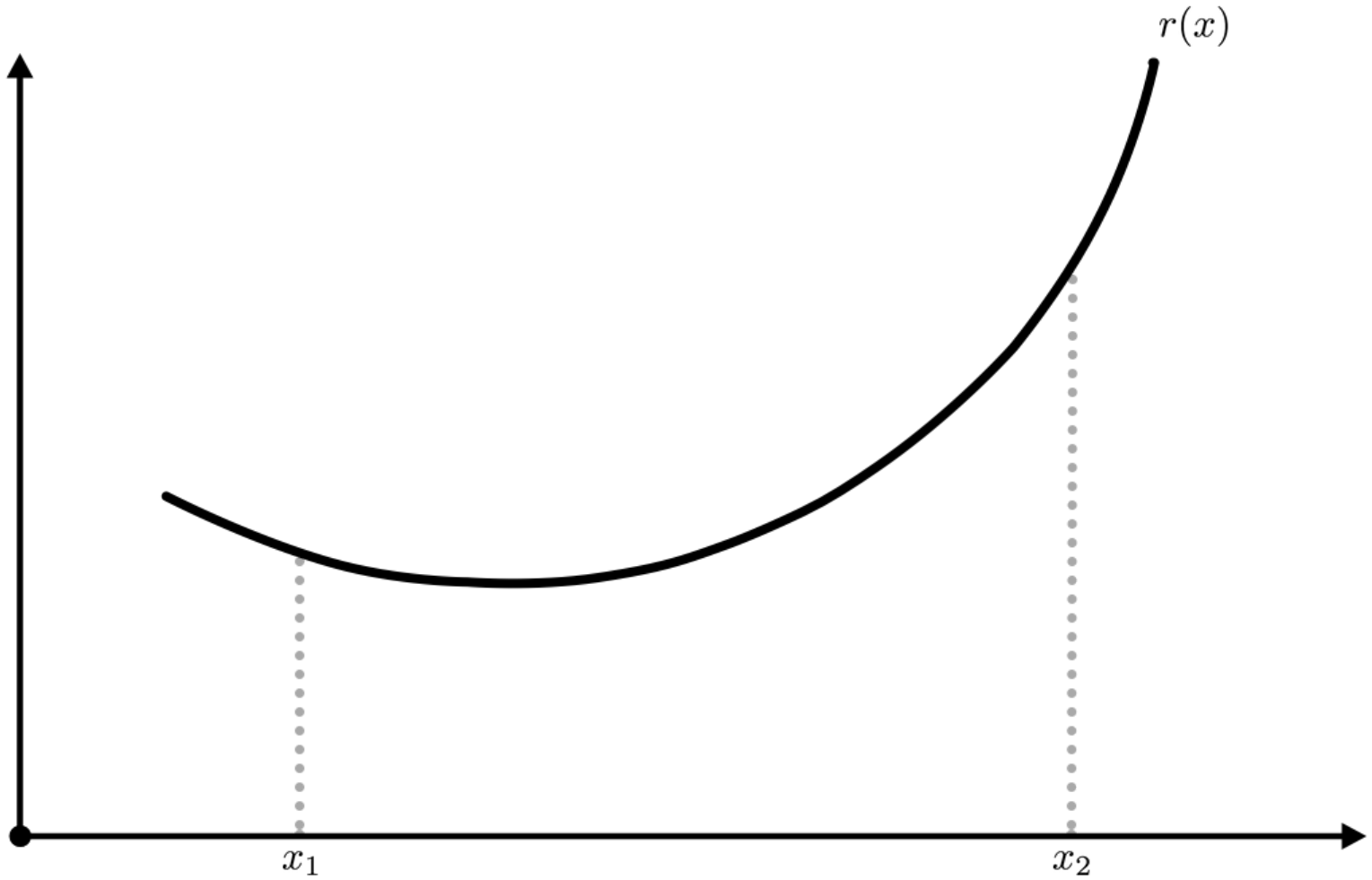

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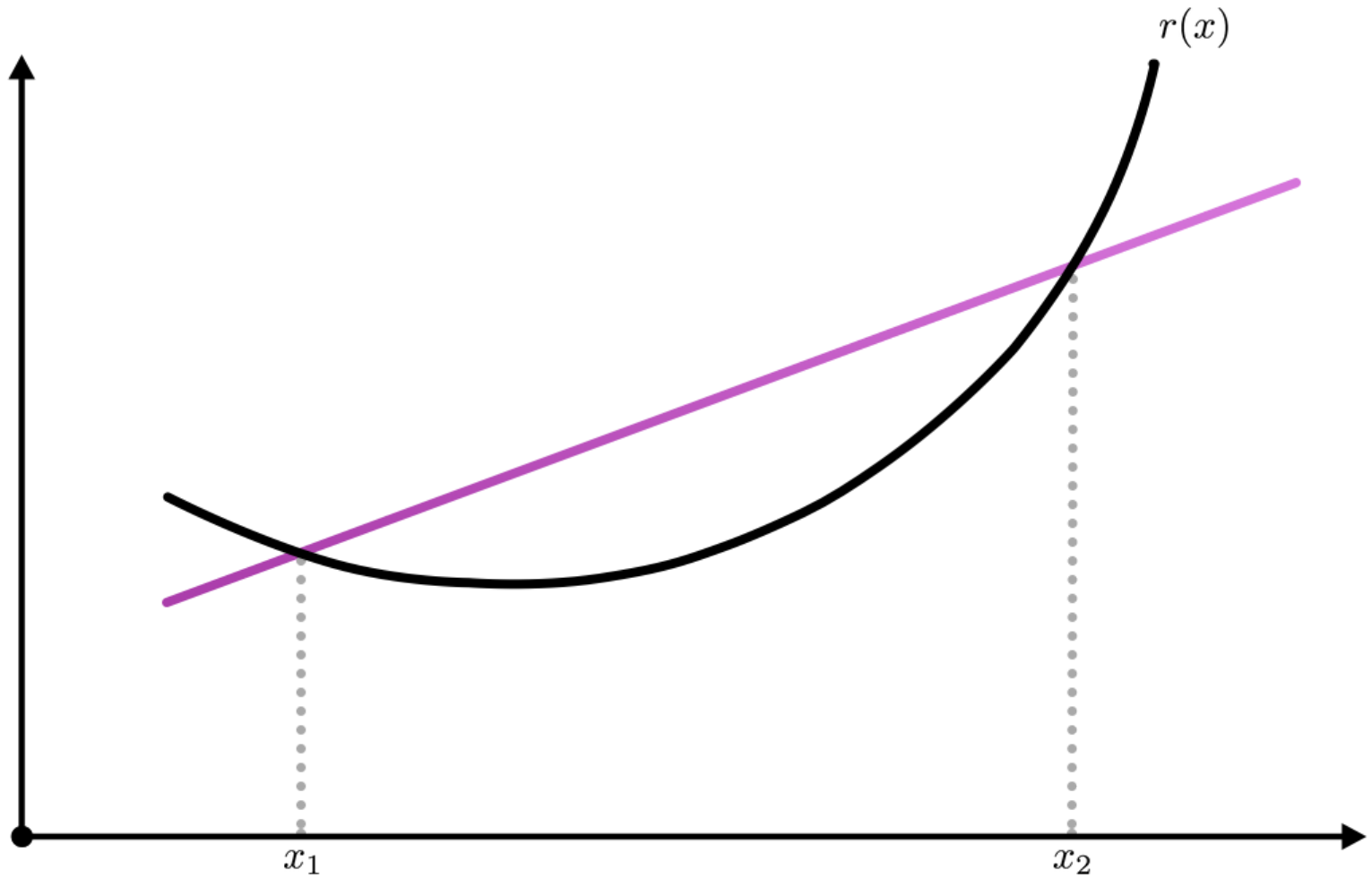

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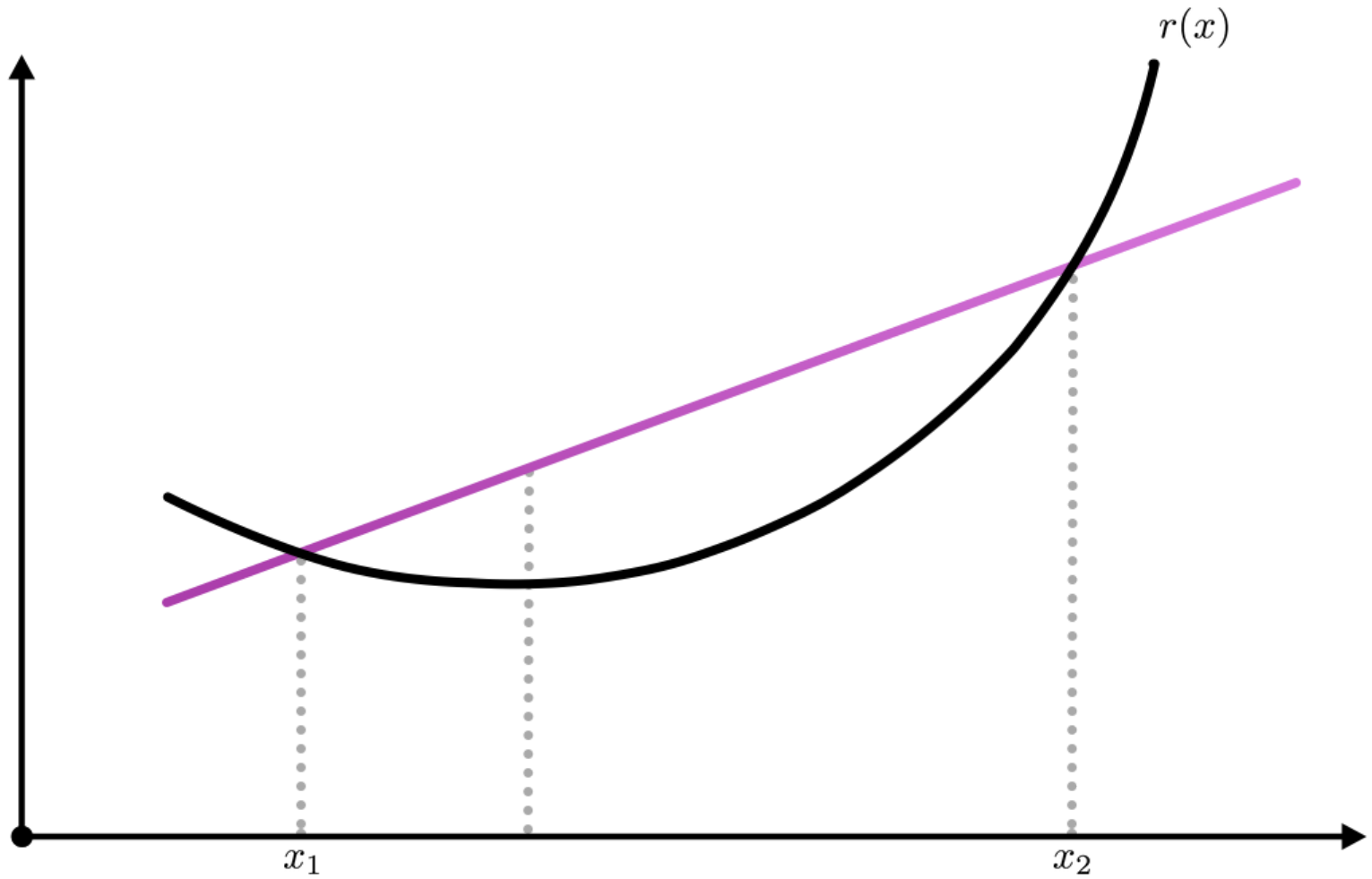

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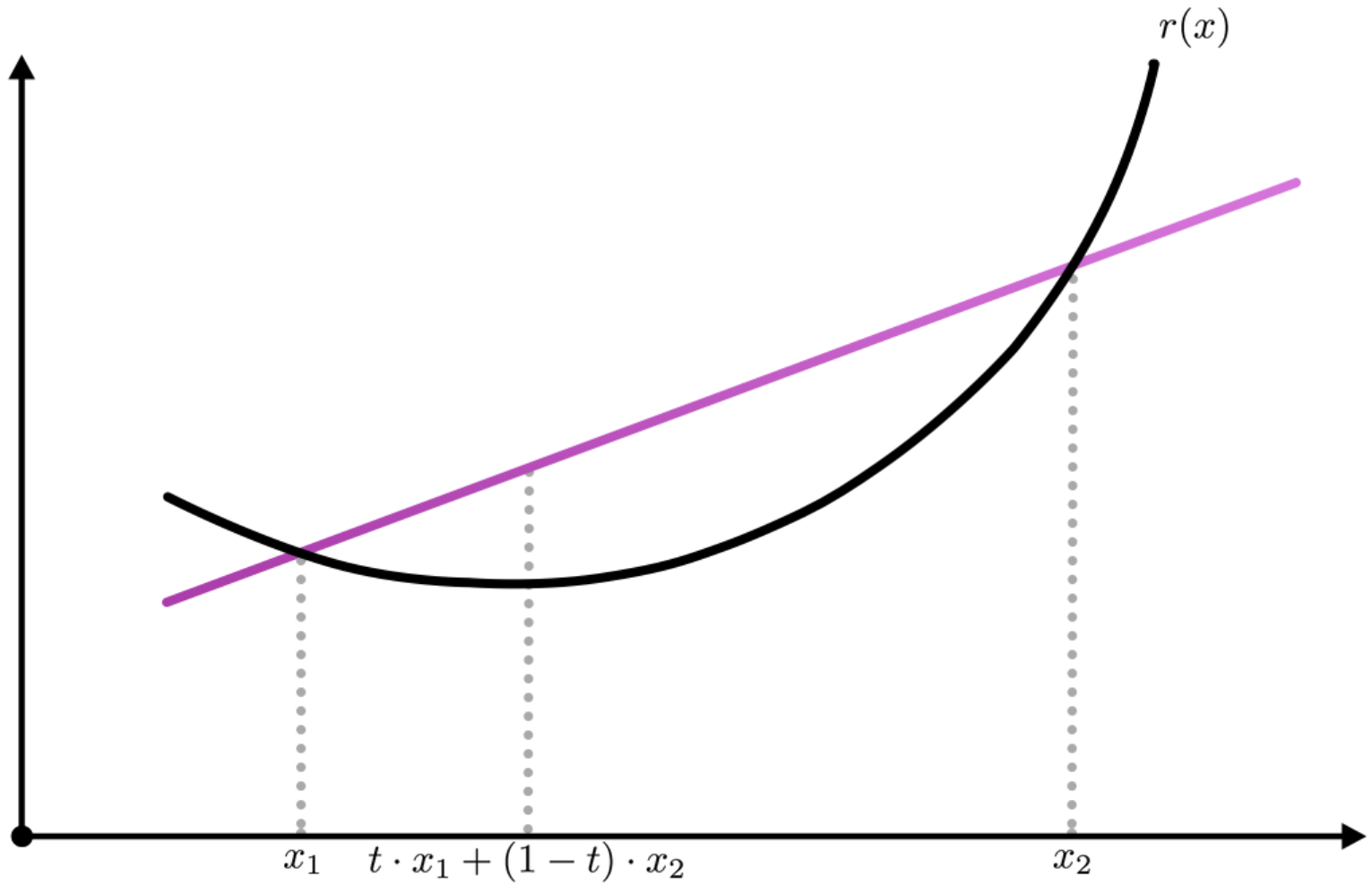
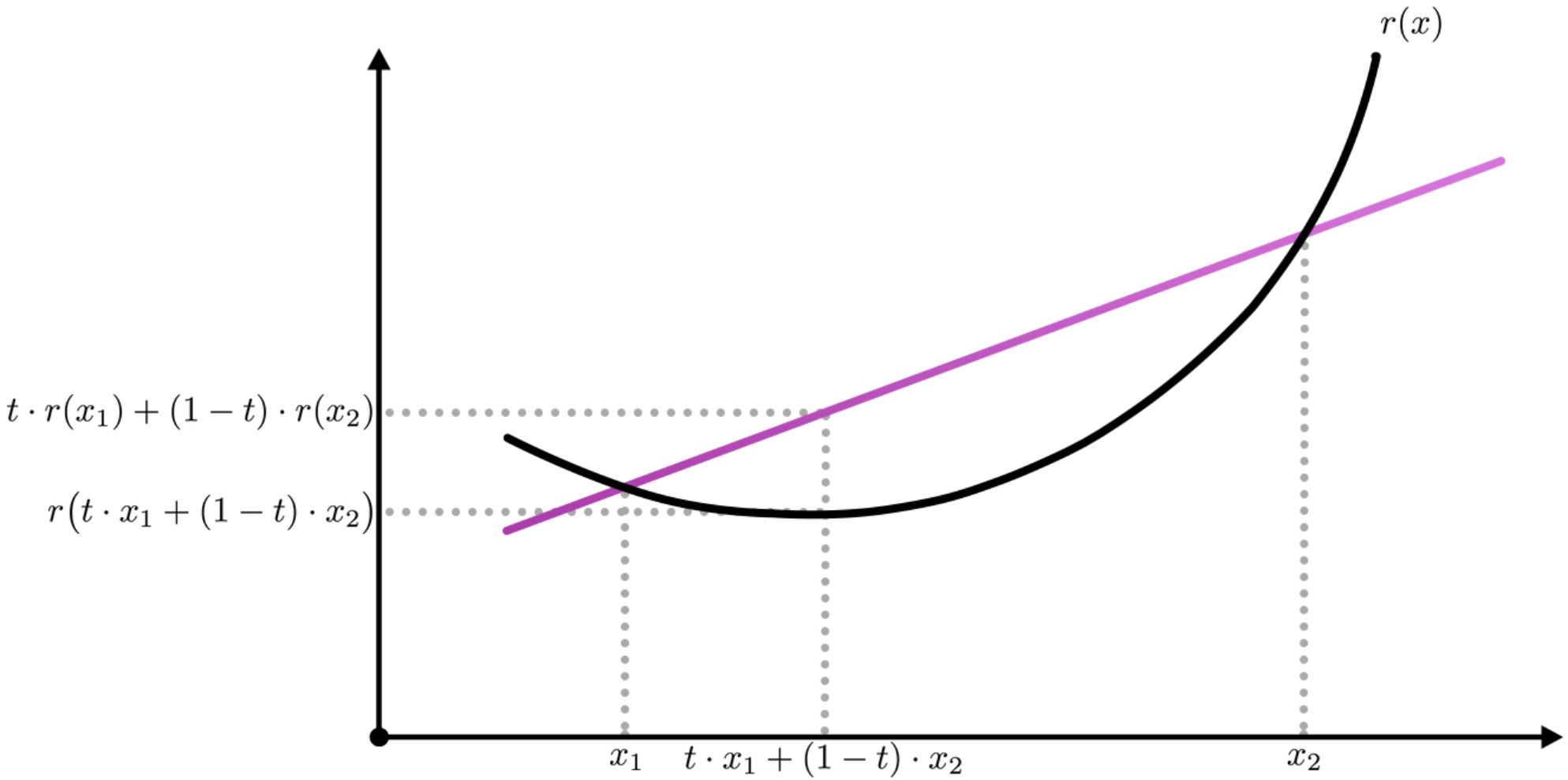


Convexity is and will be crucial



Convexity is and will be crucial

Gradient descent is basic, but powerful

- Gradient descent works well when there's a single global minimum, no flat parts to the function, and the step size is small enough to not over-shoot or zig-zag
- It's actually been re-invented a number of times under different names
  - For example, "*back-propagation*" (see Rumehlart et al., 1996)
- It's the work-horse for **large-scale** industrial applications in modern machine learning
  - Especially as **stochastic gradient descent** (see Robbins and Monro, 1951)
- It's still a bit *mysterious* why it works so well for those applications, which actually have lots of local minima!

Estimation error vs Optimization error

- For a generic ERM $\hat{s}$, remember our **approximation error** vs **estimation error** decomposition:

$$\begin{aligned} R(\hat{s}) &= R(s_{\text{opt}}) + (R(s_0) - R(s_{\text{opt}})) + (R(\hat{s}) - R(s_0)) \\ &= (\text{true minimum risk}) + (\text{approximation error from limited strategy set}) \\ &\quad + (\text{estimation error from not knowing the best-in-class set}) \end{aligned}$$

- Now we don't **even** have $\hat{s} = \operatorname{argmin} \widehat{R}(s)$, we have $\hat{s}_{\text{out}}$, the output of some algorithm

$$\begin{aligned} R(\hat{s}_{\text{out}}) &= R(s_{\text{opt}}) + (R(s_0) - R(s_{\text{opt}})) + (R(\hat{s}) - R(s_0)) + (R(\hat{s}_{\text{out}}) - R(\hat{s})) \\ &= (\text{optimal risk}) + (\text{approximation error}) + (\text{estimation error}) + (\text{optimization error}) \end{aligned}$$

- Optimization error $\approx$ what I've been calling ϵ
  - only $\approx$ because of R vs $\widehat{R}$ issue

Estimation error vs Optimization error

$$\text{risk} = \text{minimal risk} + \text{approximation error} + \text{estimation error} + \text{optimization error}$$

- Minimal risk and approximation error don't change with n or with how we optimize
- Estimation error shrinks with n: for large n, typically $O(p/n)$
  - Possibly more slowly converging in n for some families, or if p grows with n
  - *VC theory* will tell us that the *estimation error* can be $O\left(\frac{\log n/d}{n/d}\right)$
- Optimization error shrinks as we do more computational work
- There's no point to making the optimization error much smaller than the estimation error
  - More exactly: lots of work for little real benefit

Moral

Do **not** try to make the optimization error much smaller than *O(p/n)*

Do **not** bother optimizing more precisely than the noise level in the data will support

Beyond gradient descent: Newton's method

- Needing to pick the step-size a_t is annoying
- We'd like to take **big** steps, but ∇M is a local quantity and might be mis-leading far away
- **Idea**: We'd like to take **bigger** steps when the (non-zero) gradient does **not** change much
- This is **Newton's method**:

$$\theta^{(t+1)} = \theta^{(t)} - \left(\mathbf{h}(\theta^{(t)})\right)^{-1} \nabla M(\theta^{(t)})$$

  - One route to this: pretend M is quadratic, as justified by a Taylor expansion around the true minimum
- This is like gradient descent, but using the inverse Hessian to give the step size
  - And possibly a bit of rotation away from the gradient

Pros of Newton's method

$$\theta^{(t+1)} = \theta^{(t)} - \left(\mathbf{h}(\theta^{(t)})\right)^{-1} \nabla M(\theta^{(t)})$$

- **Adaptively-chosen** step size means harder to get zig-zags, over-shooting, etc.
- Need $O(\epsilon^{-2})$ steps to get an ϵ approximation to the minimum for "*nice*" functions
- For "*very nice*"functions, only need $O(\log(\log(1/\epsilon)))$ iterations
- Generally needs many **fewer** iterations than gradient descent
- Extremely useful for (approximate) **statistical inference**
  - $M(\theta) = \text{Likelihood Function}$: the *Hessian* (i.e. its curvature) is related to the *Fisher Information matrix* (it's inverse) and, consequently, to the (asymptotic) *standard error* of MLE's.
  - Hence, BFGS for example, will return the maximum likelihood estimates plus an *approximation* to their standard errors to build (asymptotic) confidence sets.

Cons of Newton's method

$$\theta^{(t+1)} = \theta^{(t)} - \left(\mathbf{h}(\theta^{(t)})\right)^{-1} \nabla M(\theta^{(t)})$$

- Hopeless if the Hessian doesn't exist or isn't invertible
- Need to take $O(p^2)$ second derivatives *and* p first derivatives, total $O(p^2)$
- Need to find $\theta^{(t+1)}$
  - Seems straightforward, it's $\theta^{(t+1)} = \theta^{(t)} - \left(\mathbf{h}(\theta^{(t)})\right)^{-1} \nabla M(\theta^{(t)})$
  - But inverting a $[p \times p]$ matrix takes $O(p^3)$ operations in general, so this would be an $O(p^3)$ step
  - Lots of variants to use approximate Hessians rather than the full deal (BFGS, built in to R's `optim()`, is one of these)

Gradient methods with big data

$$\theta^{(t+1)} = \theta^{(t)} - a_t \nabla M(\theta^{(t)})$$

$$\theta^{(t+1)} = \theta^{(t)} - \left(\mathbf{h}(\theta^{(t)})\right)^{-1} \nabla M(\theta^{(t)})$$

$$\widehat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} L(Y_i, s(X_i; \theta))$$

- Getting a value of $\widehat{R}$ at a particular θ is $O(n)$, getting $\nabla \widehat{R}$ is $O(np)$, getting $\mathbf{h}$ is $O(np^2)$
  - And that's assuming calculating $s(x_i; \theta)$ doesn't slow down with n
- Maybe OK if $n = 100$ or $n = 10^4$, but with $n = 10^9$ or $n = 10^{12}$, we really don't know which way to move

The Curses and Blessings of Dimensionality
(...in both, sampling information and model complexity...)

(...more examples to come...)

A way out: sampling is an unbiased estimate

- Pick *one* data point I at random, uniform on $1:n$
- $L\big(Y_I, s(X_I;\theta)\big)$ is random, but

$$\mathbb{E}_I\, L\big(Y_I, s(X_I;\theta)\big) = \widehat{R}(\theta)$$

- Re-brand $L\big(Y_I, s(X_I;\theta)\big)$ as $\widehat{R}_I(\theta)$

$$\begin{aligned}\mathbb{E}\widehat{R}_I(\theta) &= \widehat{R}(\theta)\\ \mathbb{E}\nabla\widehat{R}_I(\theta) &= \nabla\widehat{R}(\theta)\\ \mathbb{E}\nabla\nabla\widehat{R}_I(\theta) &= \mathbf{h}(\theta)\end{aligned}$$

Moral
Do **not** optimize with *all* the data, optimize with *random* samples

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Stochastic gradient descent

Draw *lots* of random one-point samples and let their noise cancel out

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1. Start with initial guess $\theta^{(0)}$, adjustment rate a
2. **While**: (*not too tired*) and (*making adequate progress*)

   a. $t^{\texttt{th}}$ iteration: pick random I uniformly on $1:n$

   b. **Set**:

$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \frac{a}{t} \nabla \widehat{R}_I(\theta^{(t)})$$

3. Return final θ

- **Remark**: Shrinking step-sizes by $1/t$ ensures noise in each gradient dies down

Stochastic gradient descent

$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \frac{a}{t} \nabla \widehat{R}_I(\theta^{(t)})$$

- Tons of variants:
  - Put the data points $1:n$ in a random order and then cycle through them
  - Don't check the "*making adequate progress*" condition too often
  - Adjust the $1/t$ step-size to some other function
  - **Stochastic Newton's method**: use the sample to also calculate the Hessian and take a Newton's method step
  - **Mini-batch**: sample a *few* of random data points at once
  - Mini-batch stochastic Newton's method, etc.

Pros and cons of stochastic gradient methods

- Pro: Each iteration constant (or at least constant in n)
- Pro: Never need to hold all the data in memory at once
- Pro: Does converge eventually (at least if the non-stochastic method would)
- Cons: sampling noise increases optimization error
    - That is: more iterations to come within the same ϵ of the optimum as non-stochastic GD or Newton
- Over-all pro: often low computational cost to make the optimization error small compared to the estimation error

More optimization algorithms

- Ones which play more tricks with derivatives than just gradient descent and Newton ("*conjugate gradient*", etc., etc.)
- Ones which avoid derivatives ("*simplex*" or "*Nelder-Mead*")
- Ones which avoid derivatives and try random changes ("*simulated annealing*")
- Ones which use natural-selection-with-random-variation to evolve a whole population of approximate optima ("*genetic algorithms*")

Why are there so many different optimization algorithms?

- No one algorithm works well on *every* problem
  - Sometimes obvious: don't use Newton's method if Θ is discrete
- Fundamental limit: no algorithm is *universally* better than others on *every* problem (**no free lunch theorem** of Wolpert et al., 1997)
  - For every problem where your favorite algorithm does better than mine, I can design a new problem where my algorithm leads by just as much (see Culberson, 1998)
- We need to know *something* about the problem to select a good optimizer

Summing up

- With real data and real computers, finding the empirical-risk-minimizer means using an algorithm to solve an optimization problem
- These algorithms almost never give the **exact** optimum but just an *approximation*
- Usually, the longer an algorithm is allowed to work, the closer it can get to the true optimum
- This adds **optimization error** on to *estimation error*
- For *many* statistical learning problems, gradient descent and Newton's method work really well
    - With **sampling** to make them more computationally efficient for big data
- Don't bother reducing the optimization error much *beyond* the estimation error
- **No** algorithm is best for all problems
- **Coming up**:

    1. More on Convexity
    2. *Constrained* Optimization $\rightsquigarrow$ Lagrange Multipliers + Duality