lecture 6: differentiation

deep learning for vision

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outline

gradient descent
gradient computation
automatic differentiation: units
automatic differentiation: functions
fun

gradient descent

gradient descent

- a first-order Taylor approximation of $f : \mathbb{R}^d \to \mathbb{R}$ at $\mathbf{x}_0$ is

$$f^{(1)}_{\mathbf{x}_0}(\mathbf{x}) := f(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0)^\top \nabla f(\mathbf{x}_0)$$

  i.e. , the gradient points in the direction of the greatest increase rate

- a second-order approximation needs the Hessian matrix Hf

$$f^{(2)}_{\mathbf{x}_0}(\mathbf{x}) := f^{(1)}_{\mathbf{x}_0}(\mathbf{x}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^\top (Hf(\mathbf{x}_0))(\mathbf{x} - \mathbf{x}_0)$$

- assuming f is locally convex with isotropic $Hf(\mathbf{x}_0) = \frac{1}{\epsilon} I$, the gradient of $f^{(2)}_{\mathbf{x}_0}$ is

$$\nabla f^{(2)}_{\mathbf{x}_0}(\mathbf{x}) = \nabla f(\mathbf{x}_0) + \frac{1}{\epsilon}(\mathbf{x} - \mathbf{x}_0)$$

- so if we were to minimize this approximation instead of f,

$$\arg\min_{\mathbf{x}} f^{(2)}_{\mathbf{x}_0}(\mathbf{x}) = \mathbf{x}_0 - \epsilon \nabla f(\mathbf{x}_0)$$

gradient descent

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gradient descent

- this yields the update rule

$$\mathbf{x}^{(\tau+1)} = \mathbf{x}^{(\tau)} - \epsilon \nabla f(\mathbf{x}^{(\tau)})$$

i.e. , we are moving in the direction of the greatest decrease rate such that locally (depending on ϵ)

$$\begin{aligned} f^{(1)}_{\mathbf{x}^{(\tau)}}(\mathbf{x}^{(\tau+1)}) &= f(\mathbf{x}^{(\tau)}) + (\mathbf{x}^{(\tau+1)} - \mathbf{x}^{(\tau)})^\top \nabla f(\mathbf{x}_0) \\ &= f(\mathbf{x}^{(\tau)}) - \epsilon \nabla f(\mathbf{x}_0)^\top \nabla f(\mathbf{x}_0) \\ &\leq f(\mathbf{x}^{(\tau)}) \end{aligned}$$

- the step size ϵ is inversely proportional to the curvature we assume for f at the local minimum

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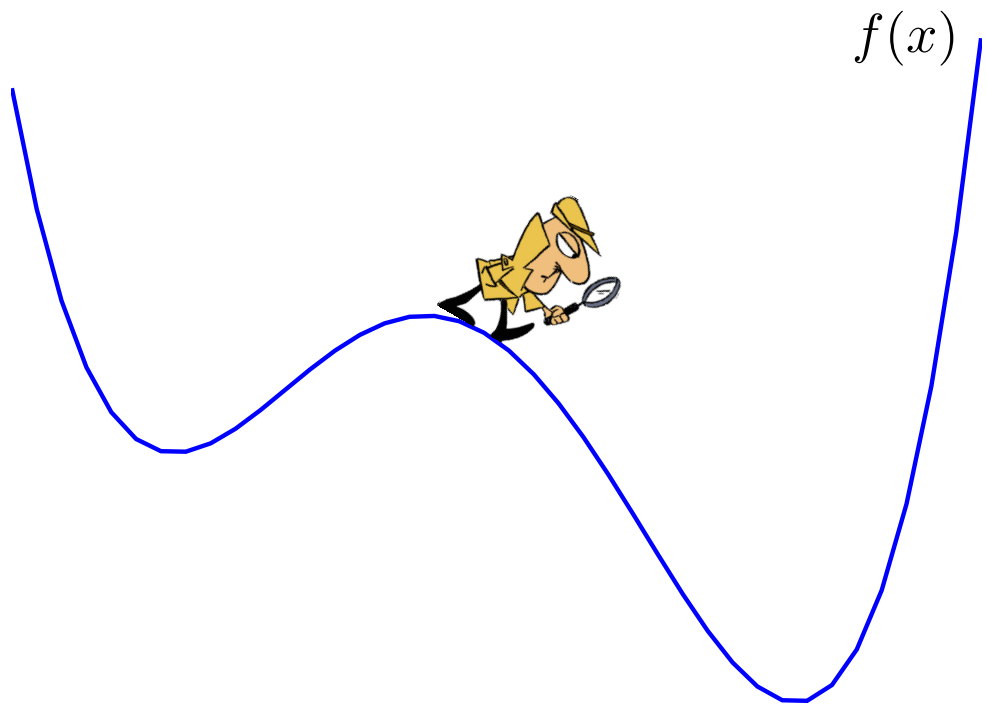
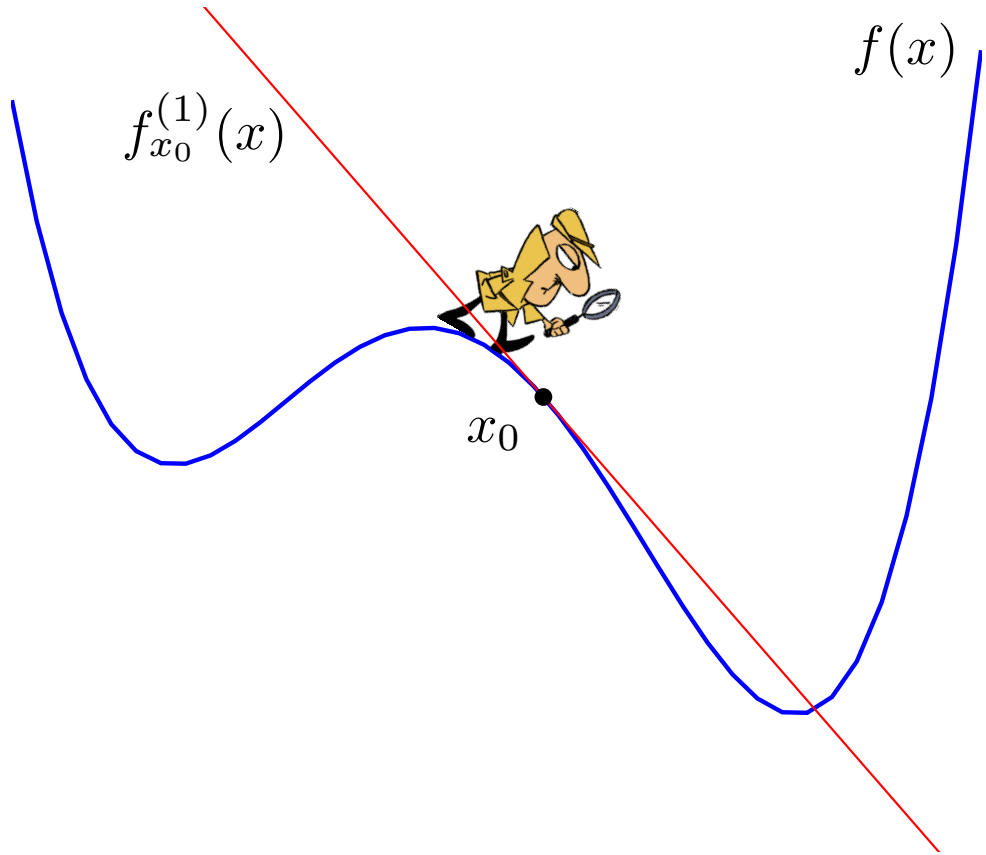
gradient descent in one dimension



- $\epsilon = 0.05$: converges to local minimum

Artwork credit: `https://the-fox-after-dark.deviantart.com/`

gradient descent in one dimension



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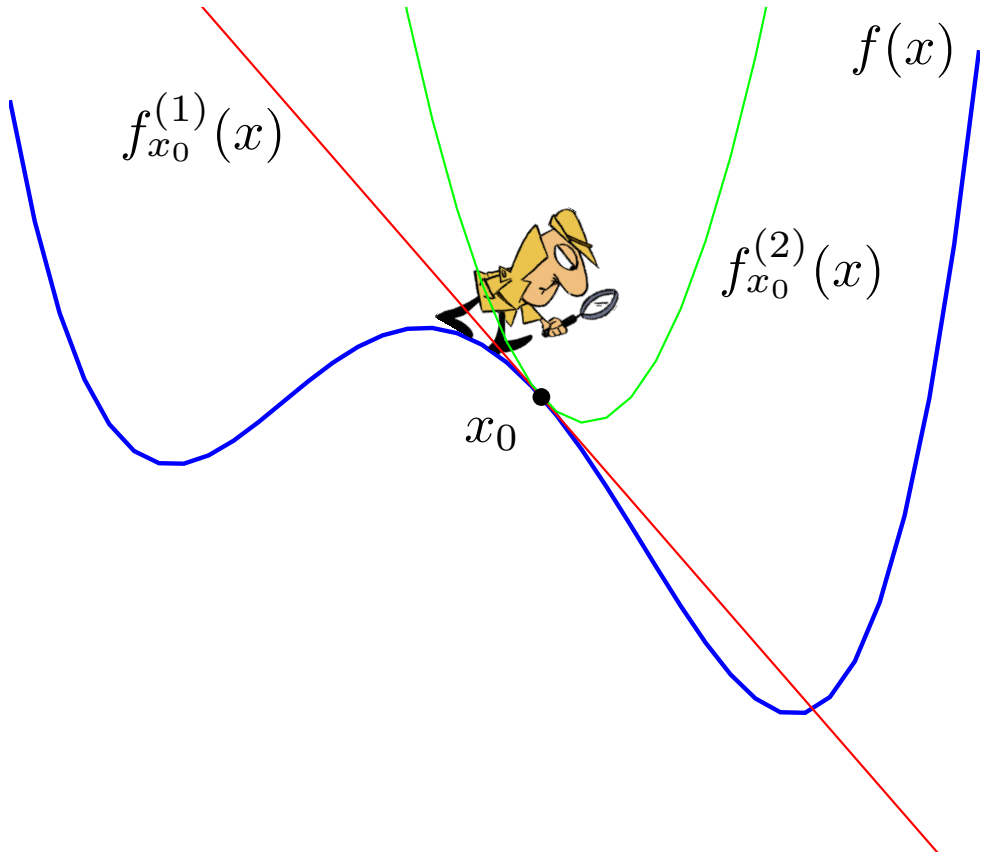
gradient descent in one dimension



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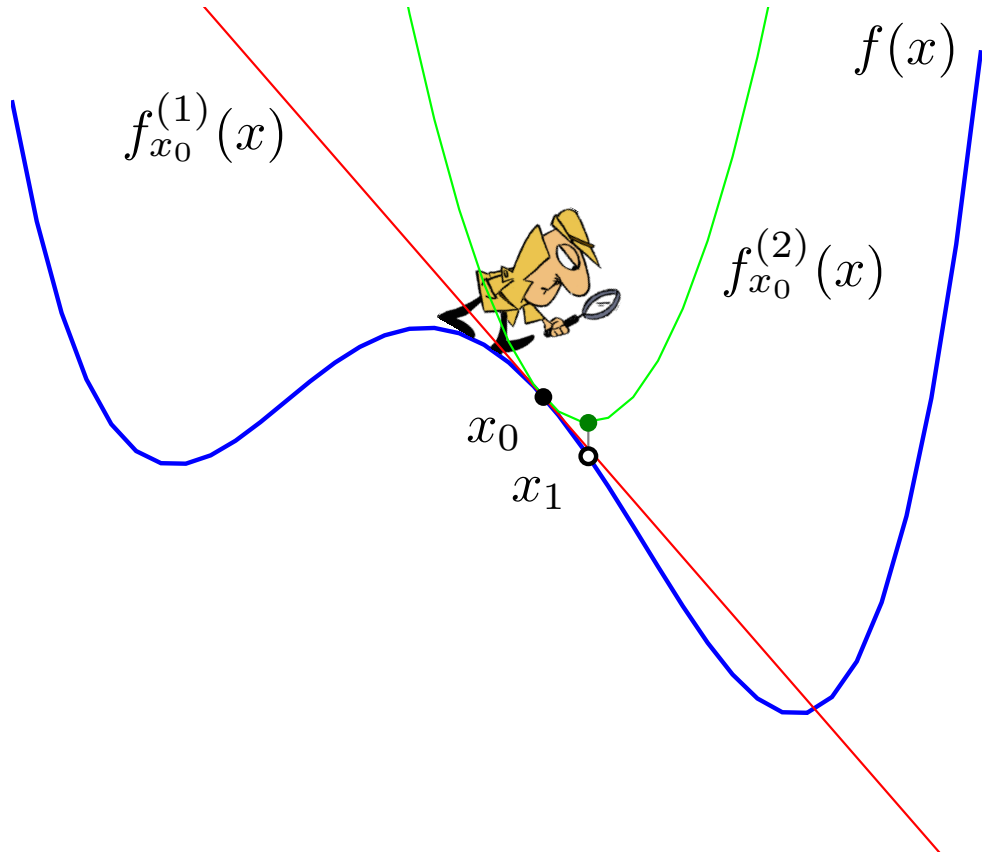

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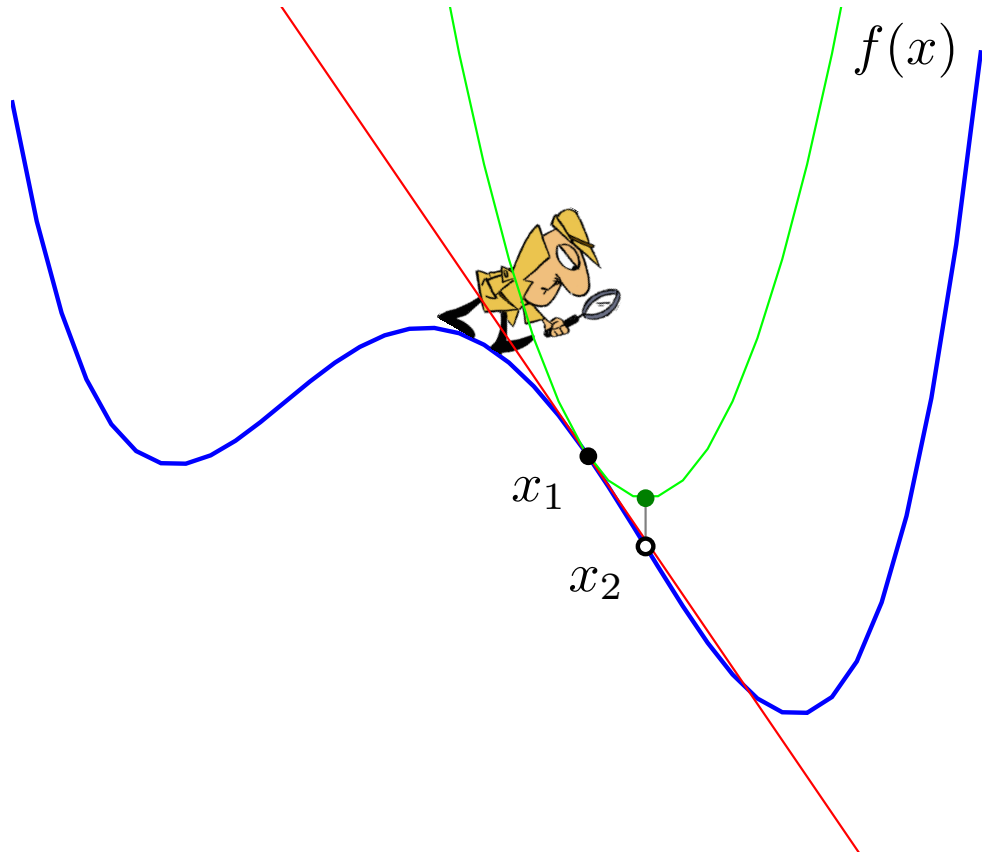

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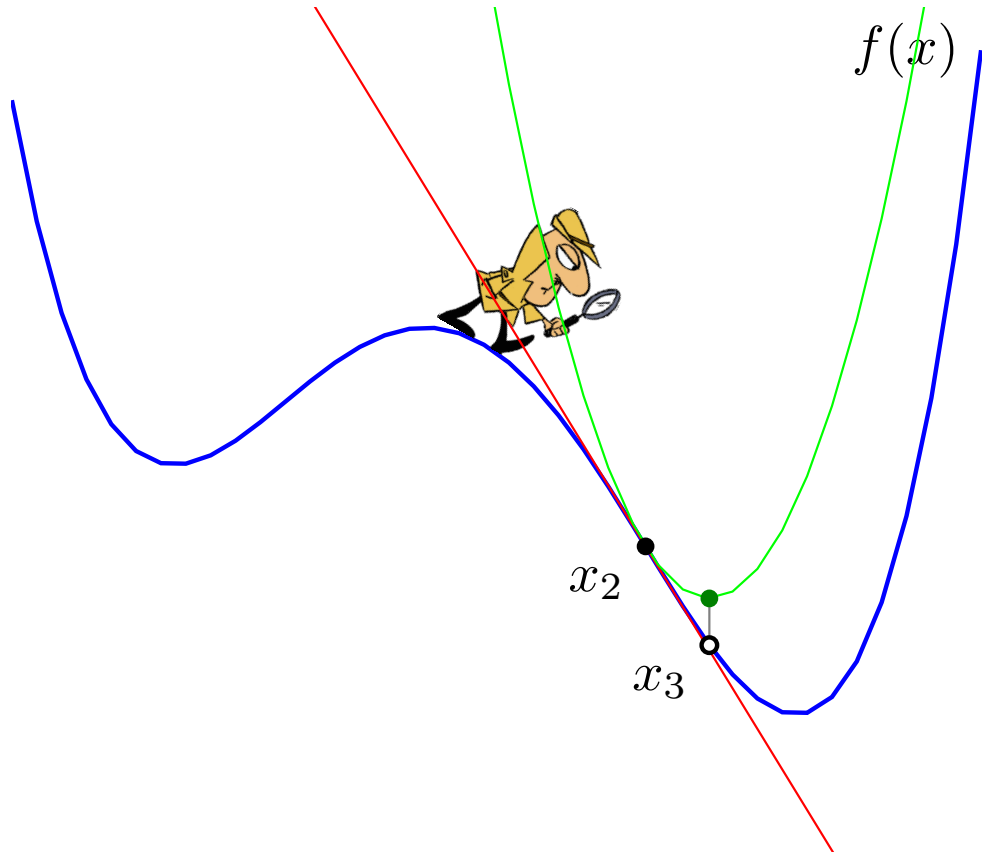
gradient descent in one dimension



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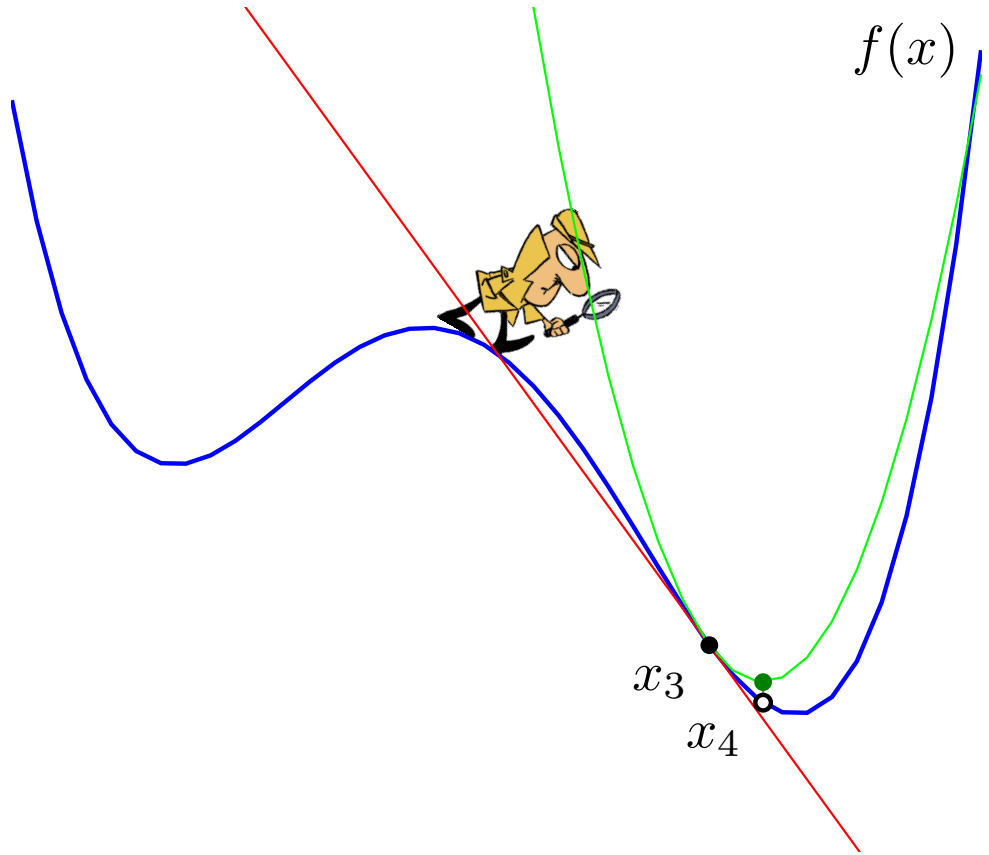

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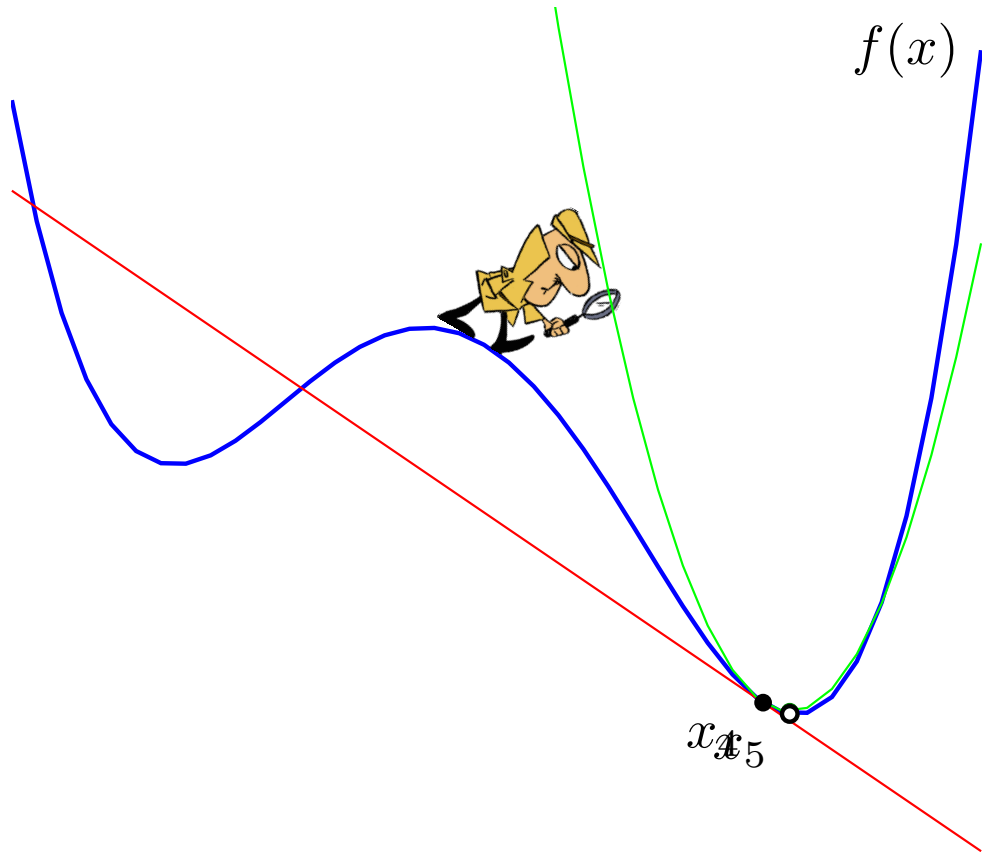
gradient descent in one dimension



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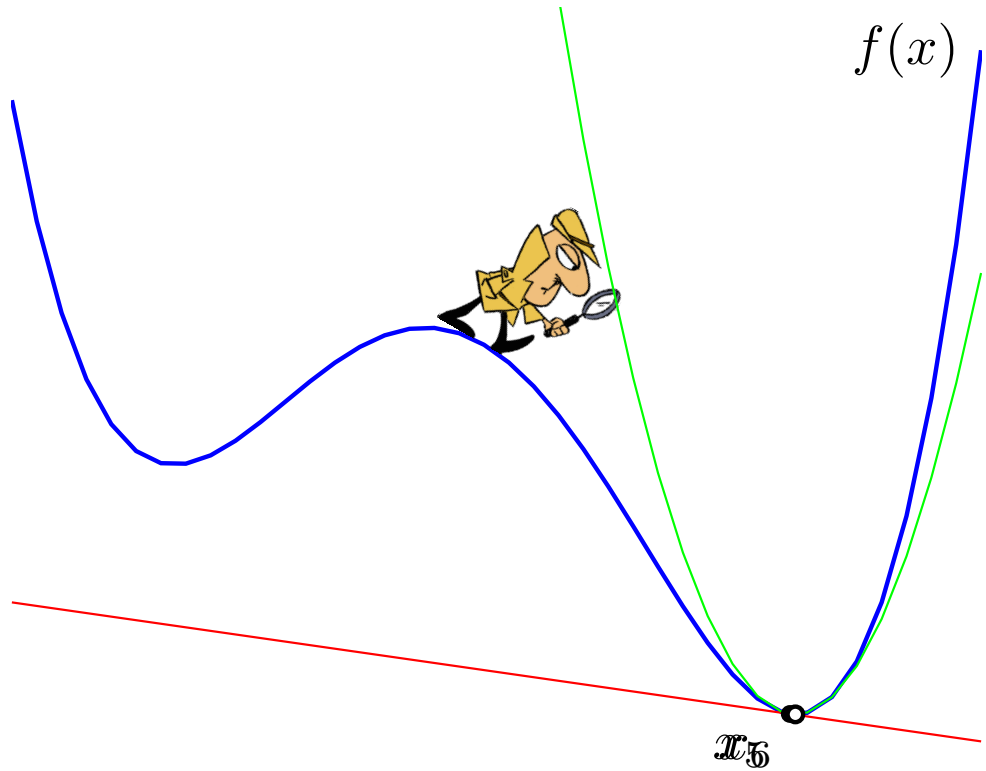

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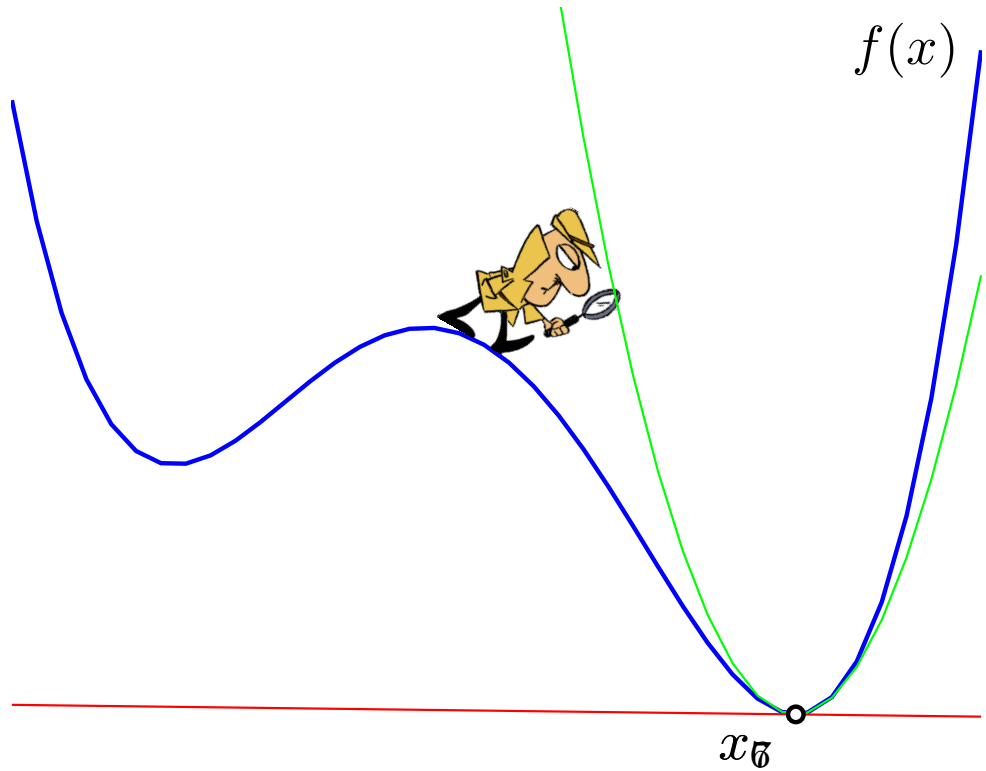

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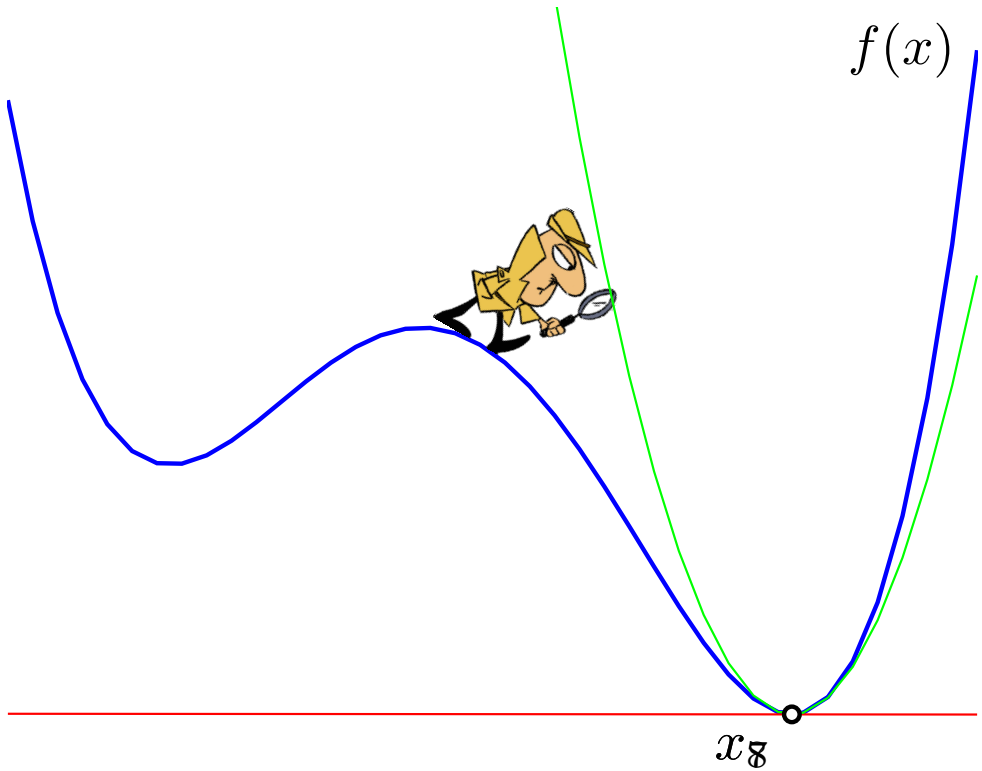

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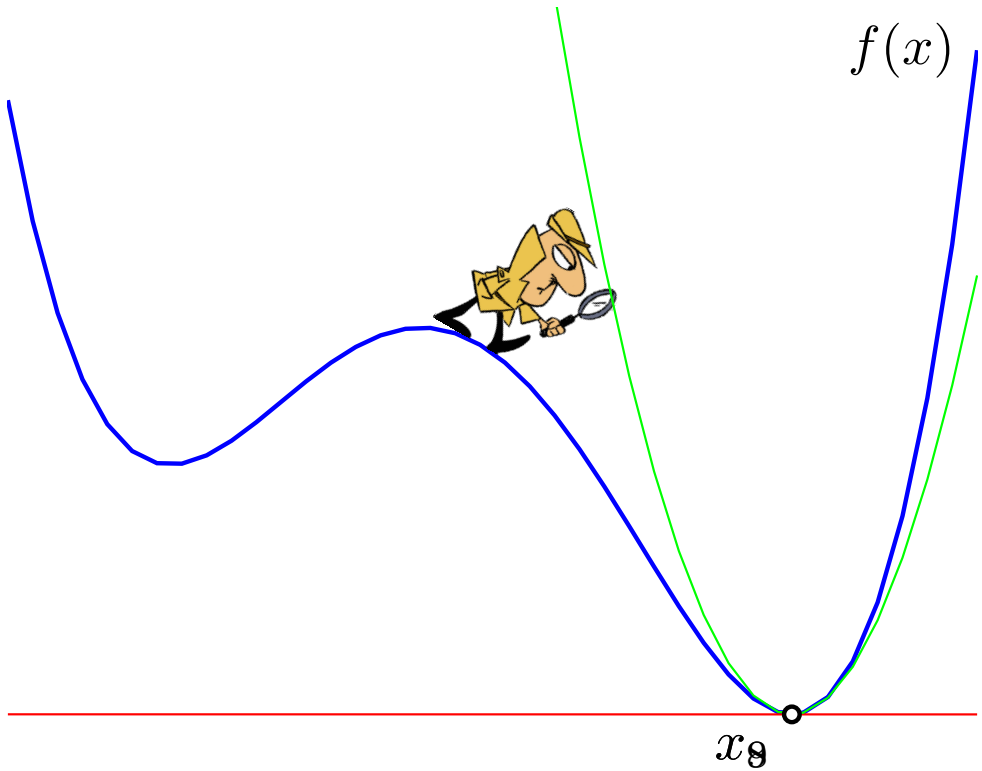
gradient descent in one dimension



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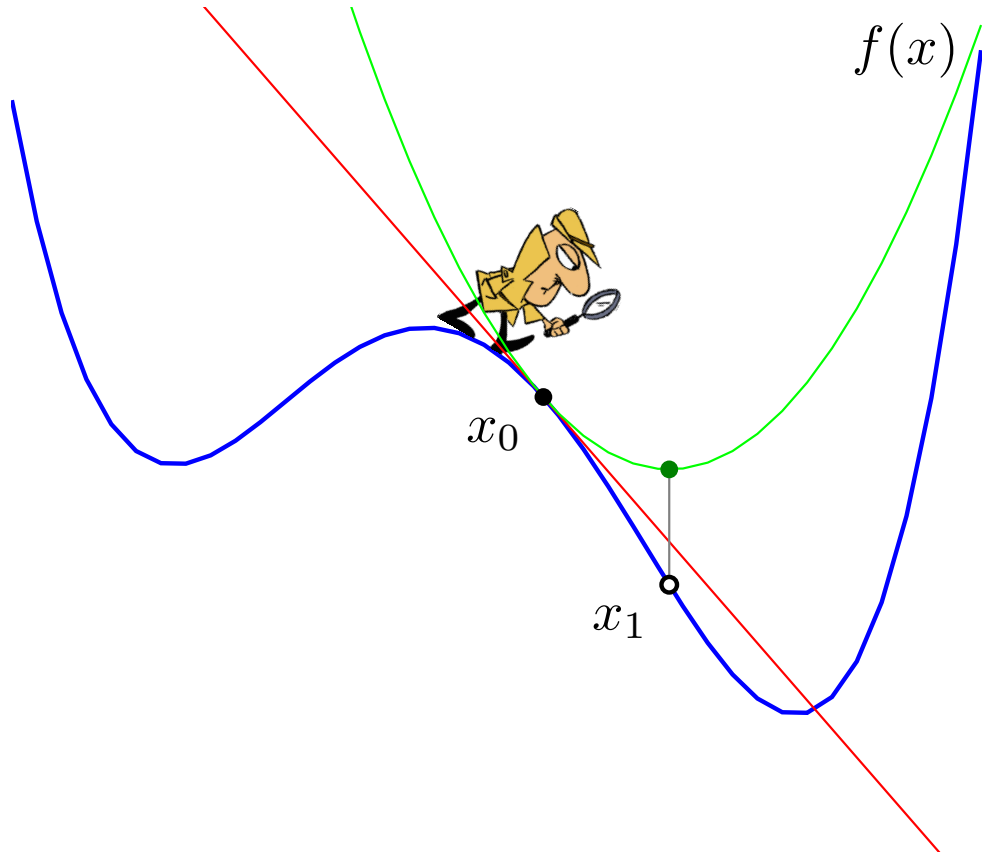

- $\epsilon = 0.14$: $1/\epsilon$ less than actual curvature, does not converge

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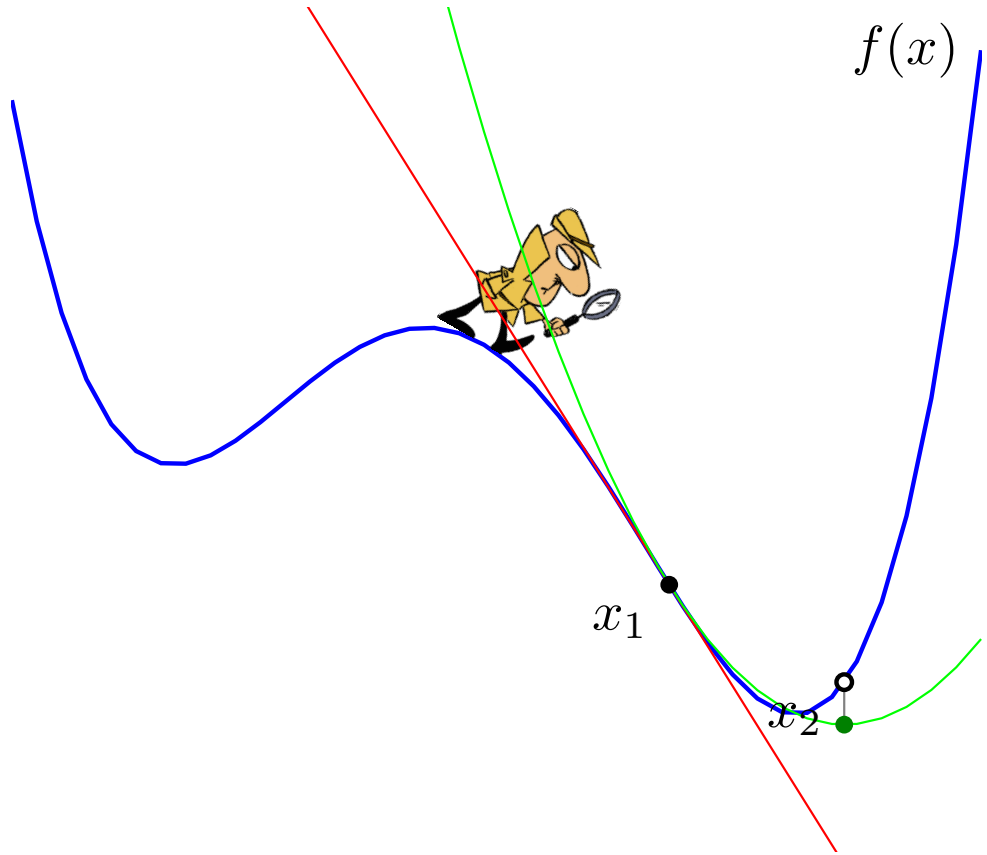
gradient descent in one dimension



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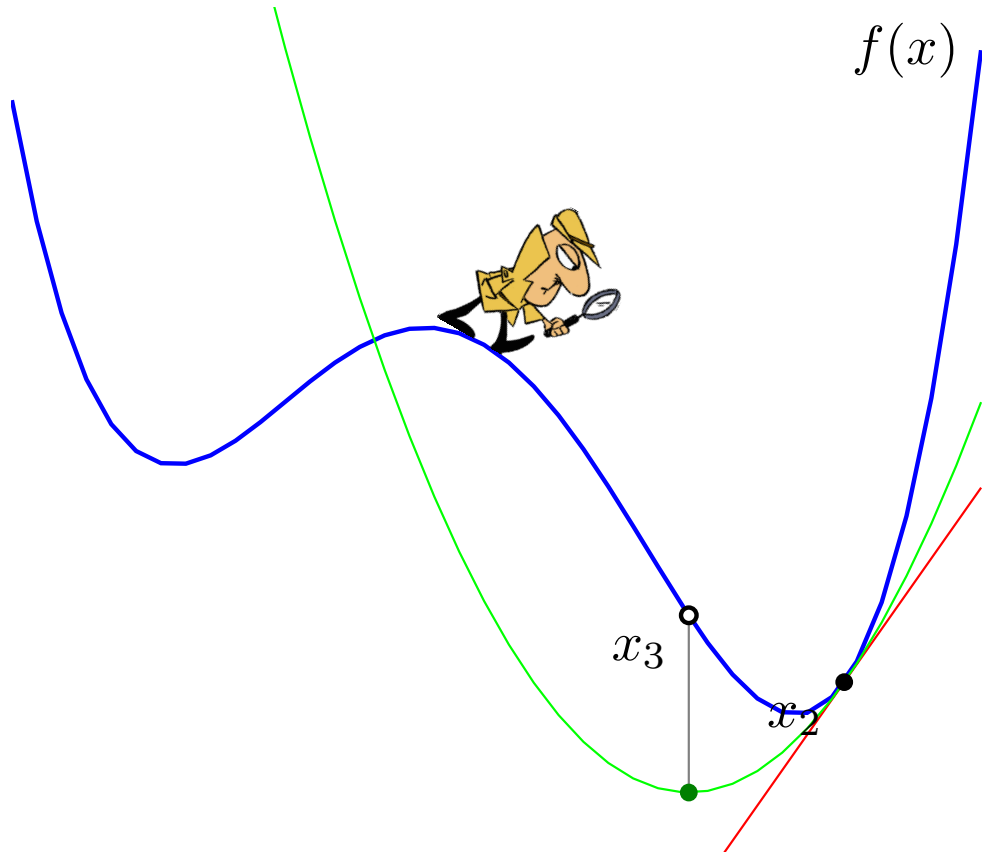

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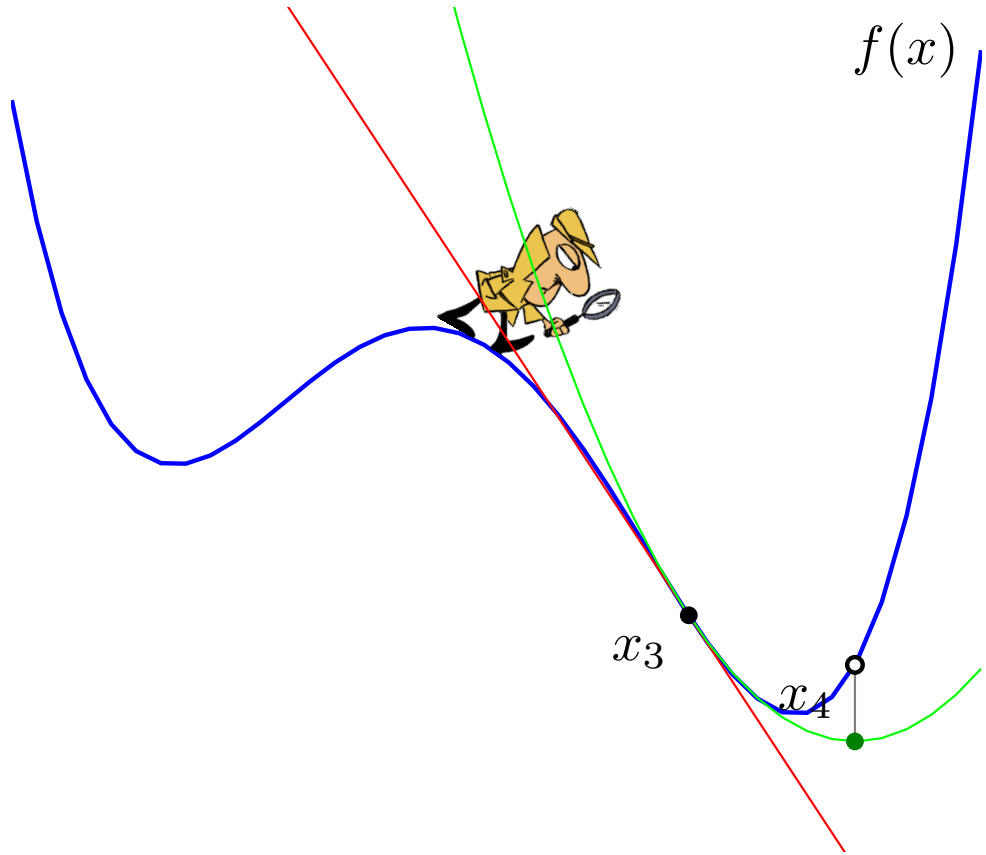

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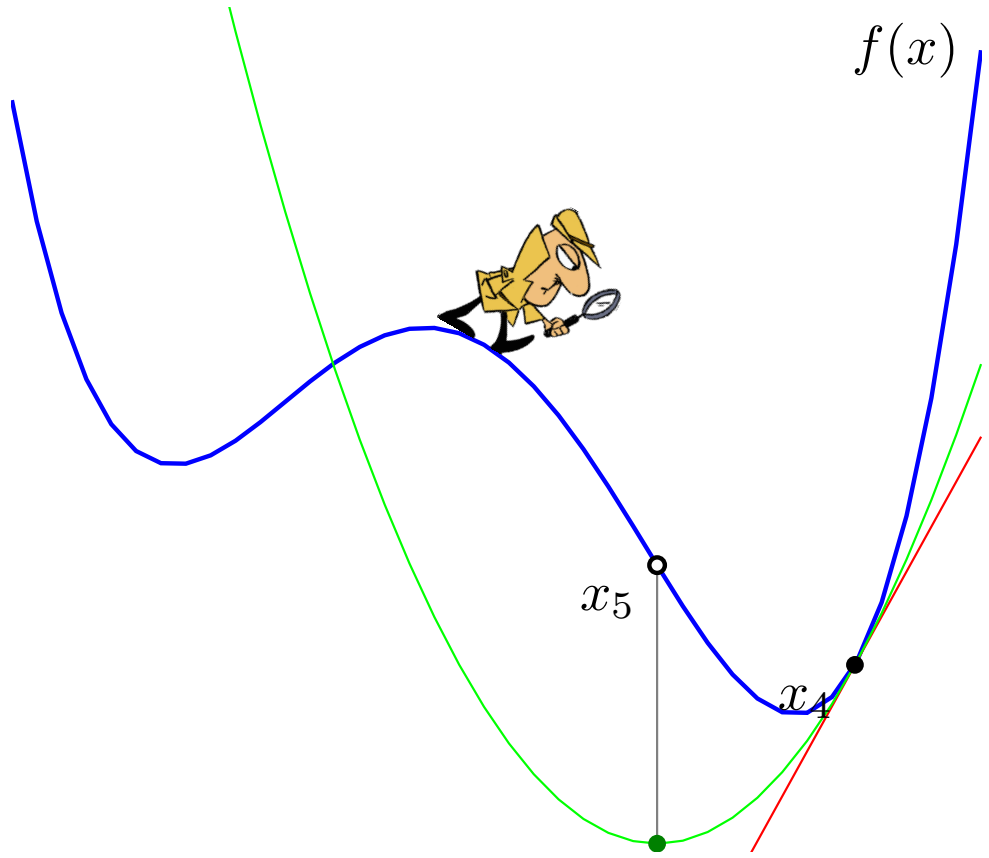

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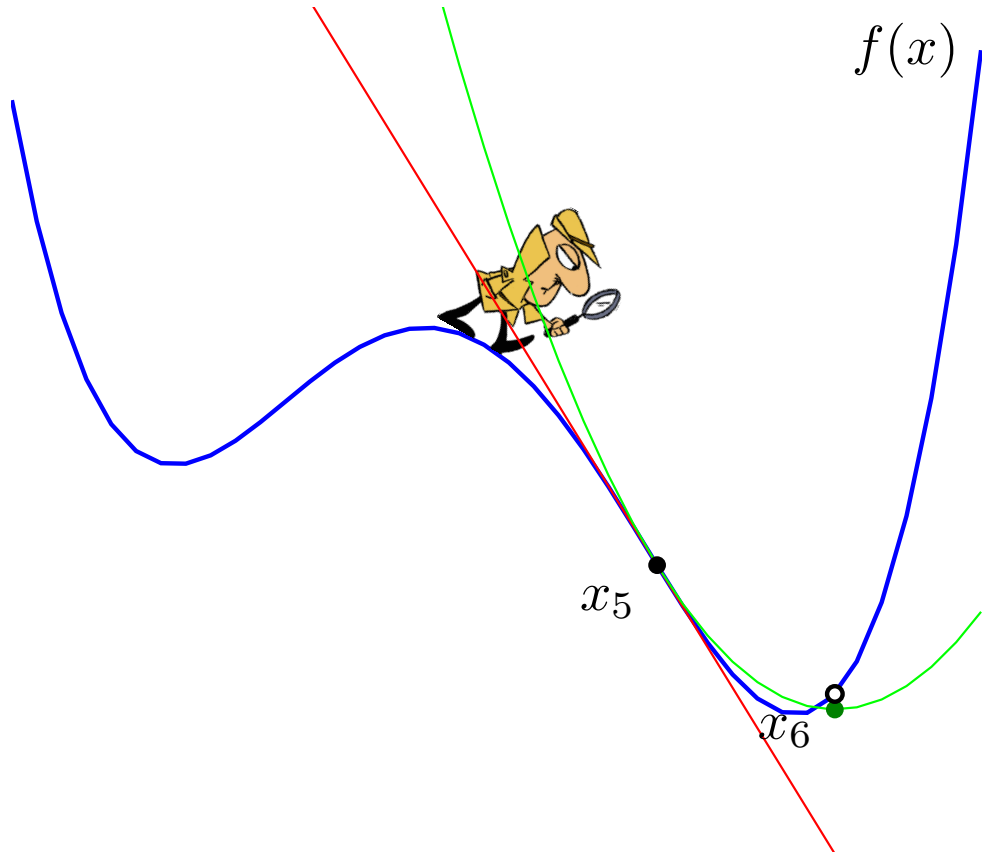

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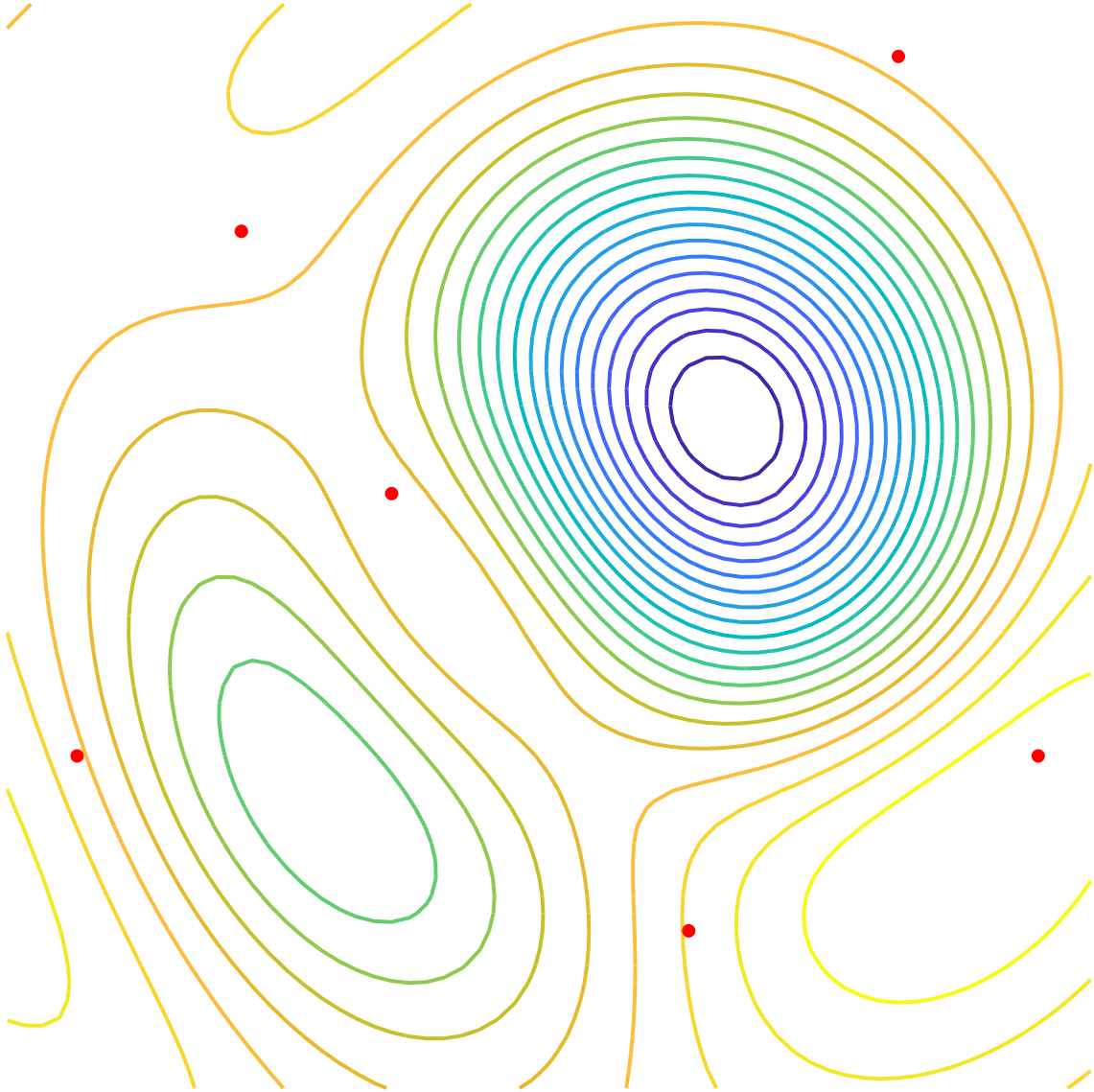
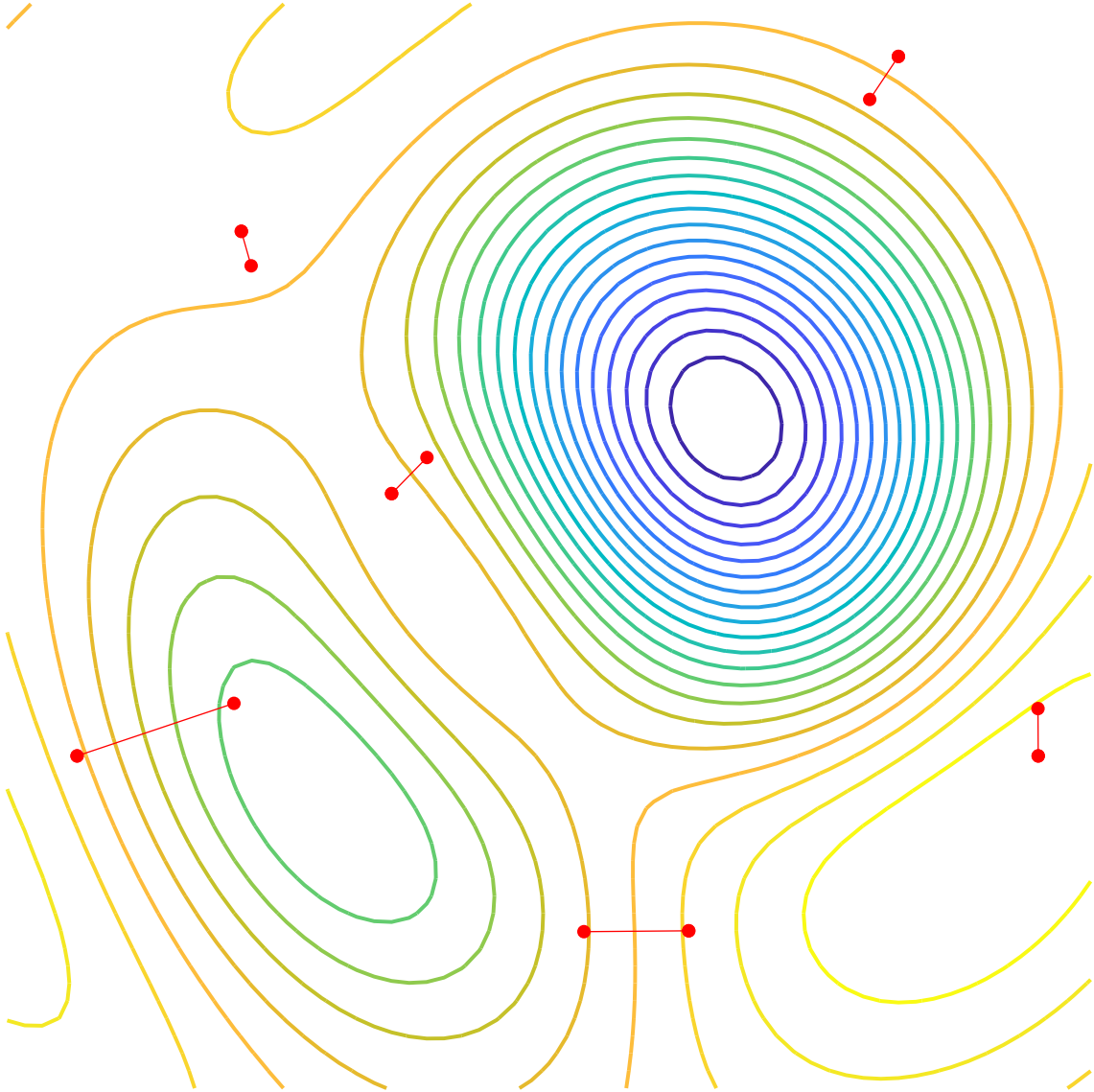
Artwork credit: https://the-fox-after-dark.deviantart.com/

gradient descent in two dimensions



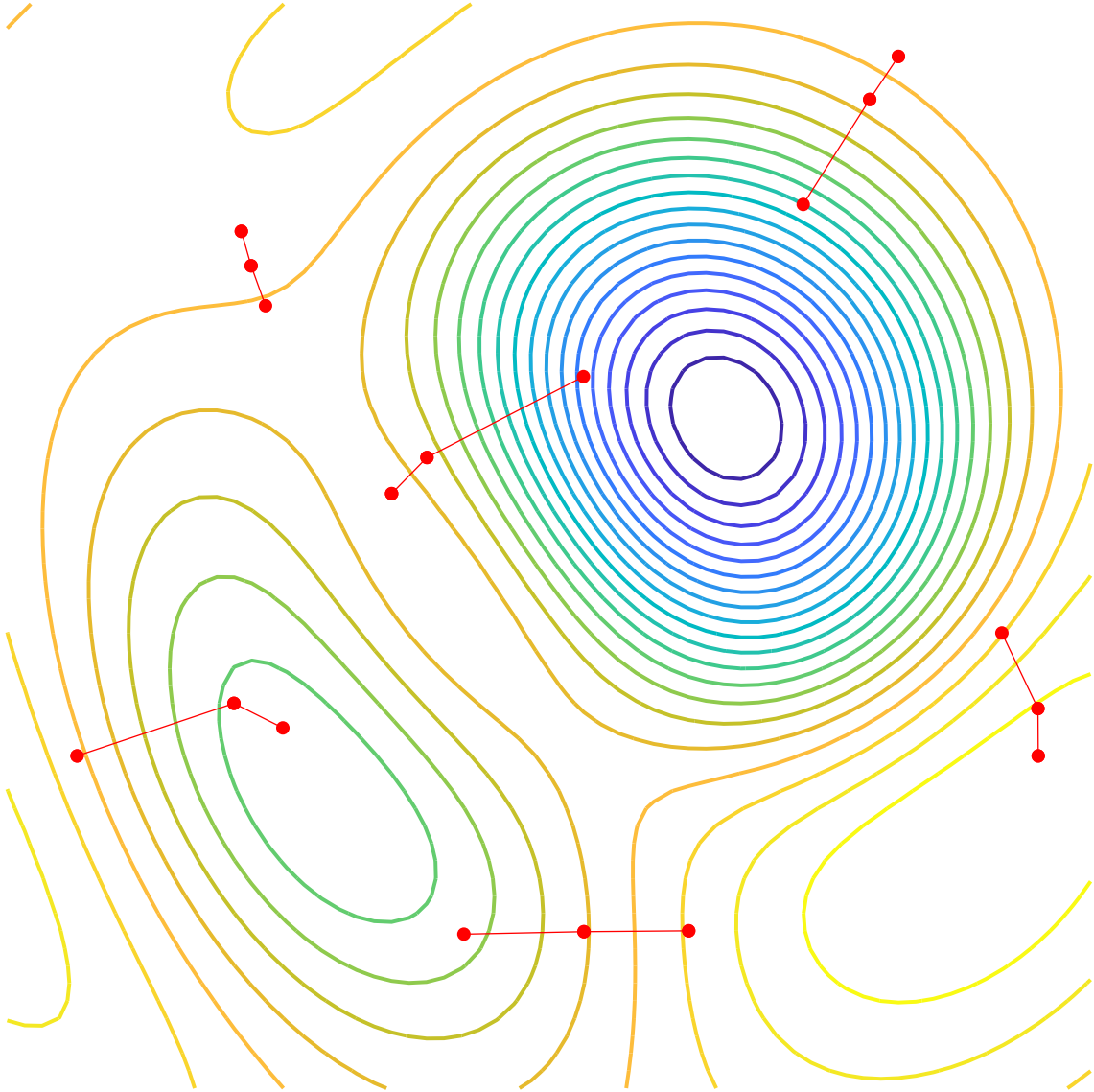
$\epsilon = 0.14$, iteration 0

gradient descent in two dimensions



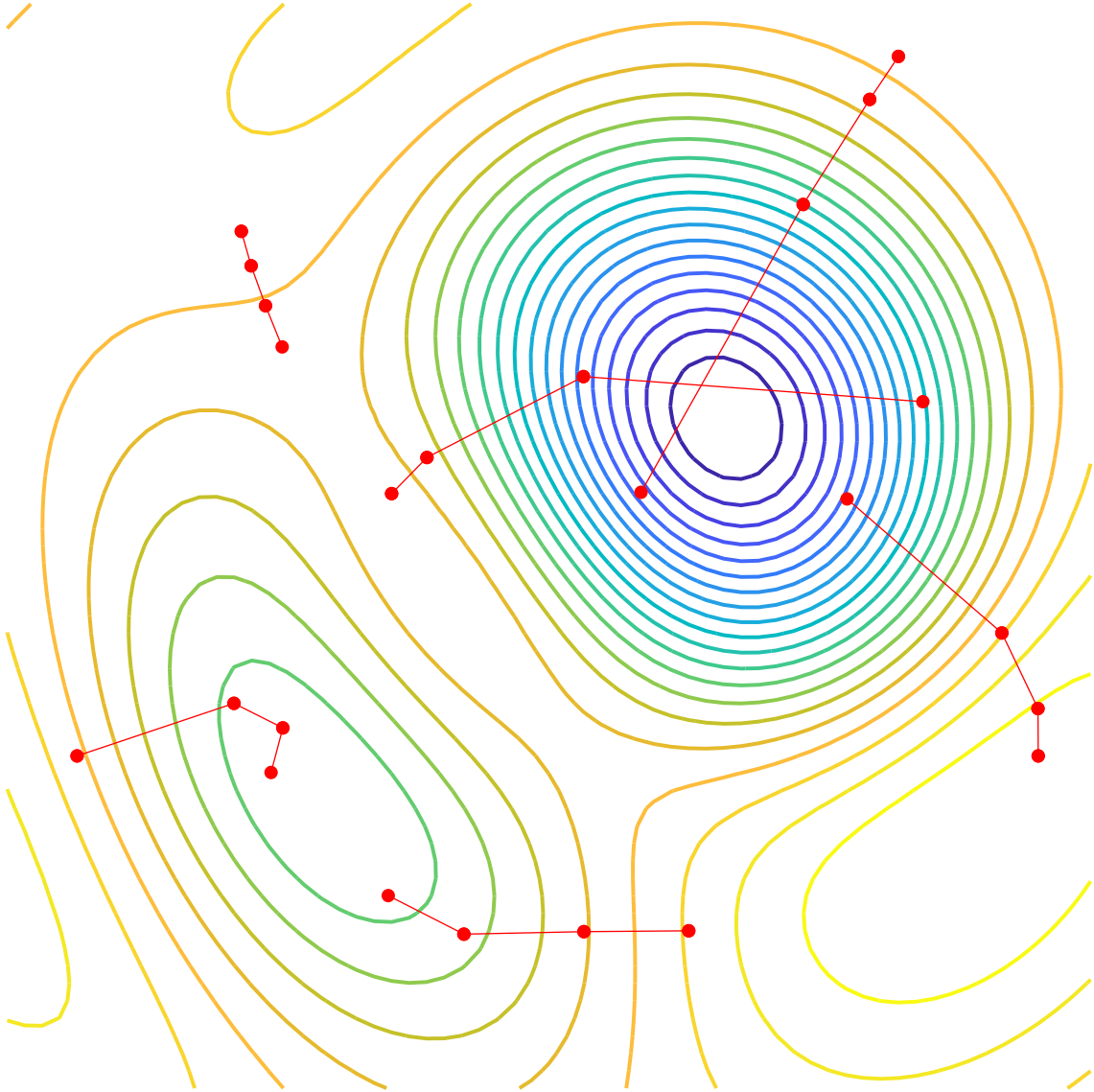
$\epsilon = 0.14$, iteration 1

gradient descent in two dimensions



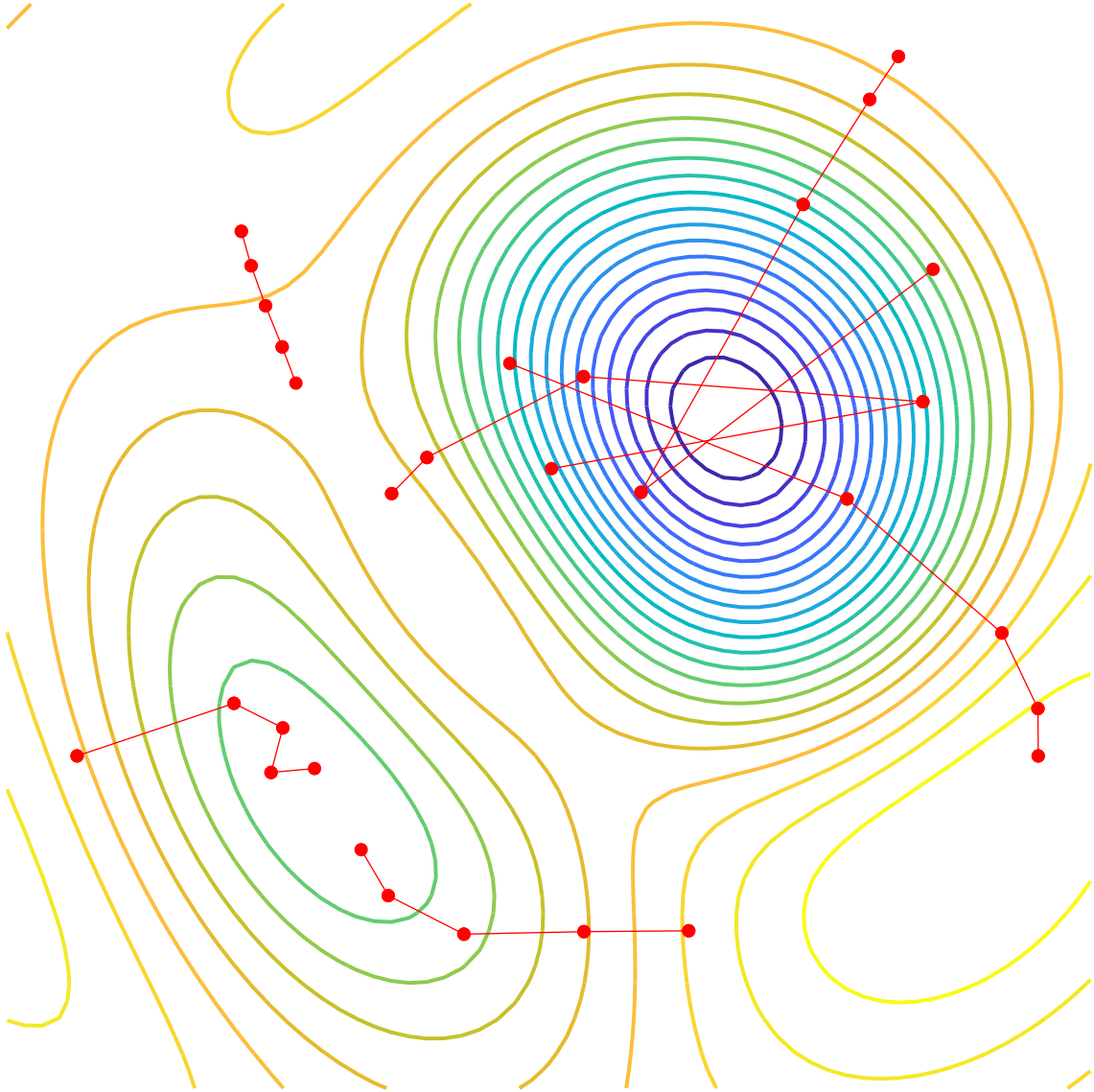
$\epsilon = 0.14$, iteration 2

gradient descent in two dimensions



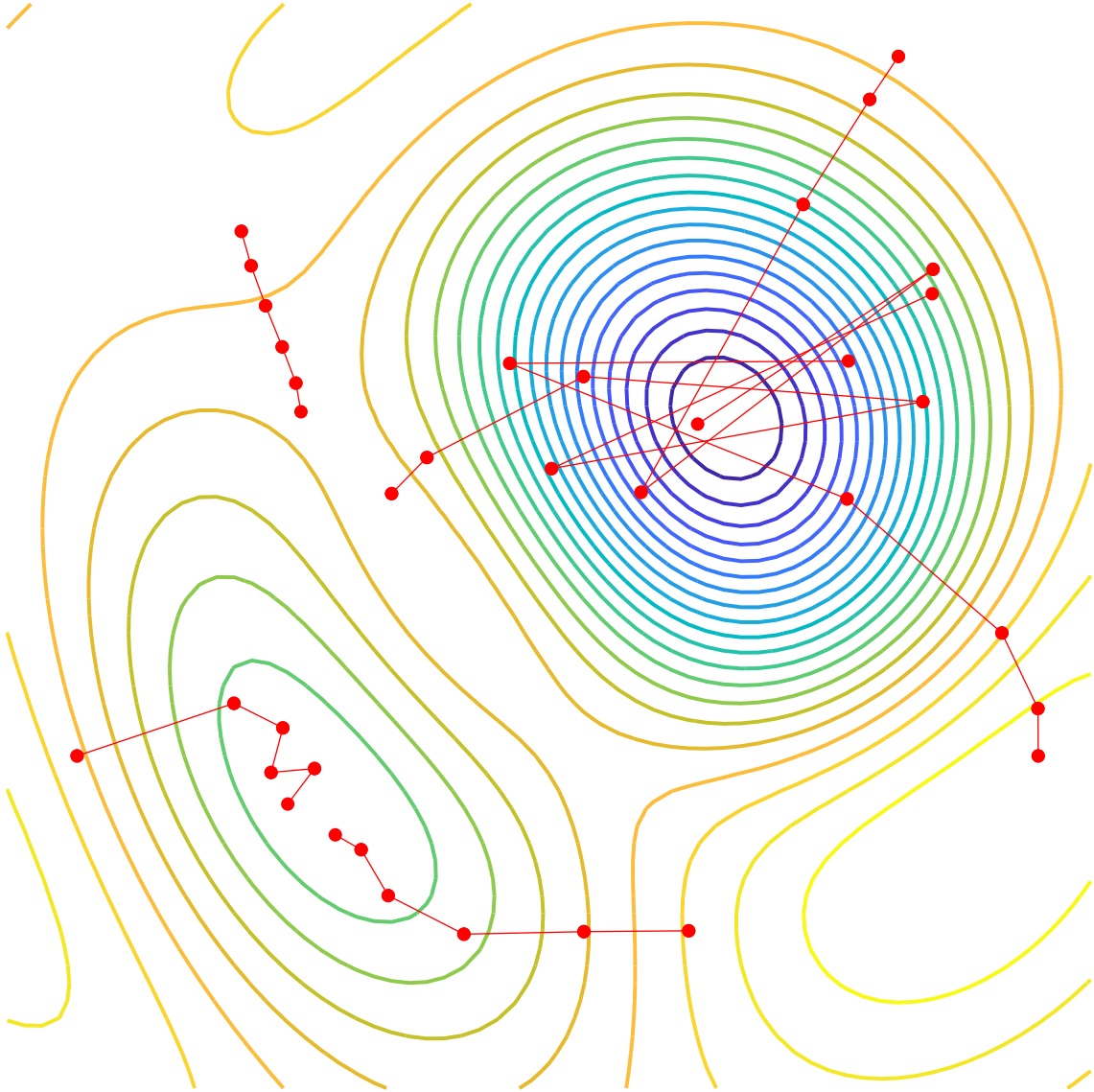
$\epsilon = 0.14$, iteration 3

gradient descent in two dimensions



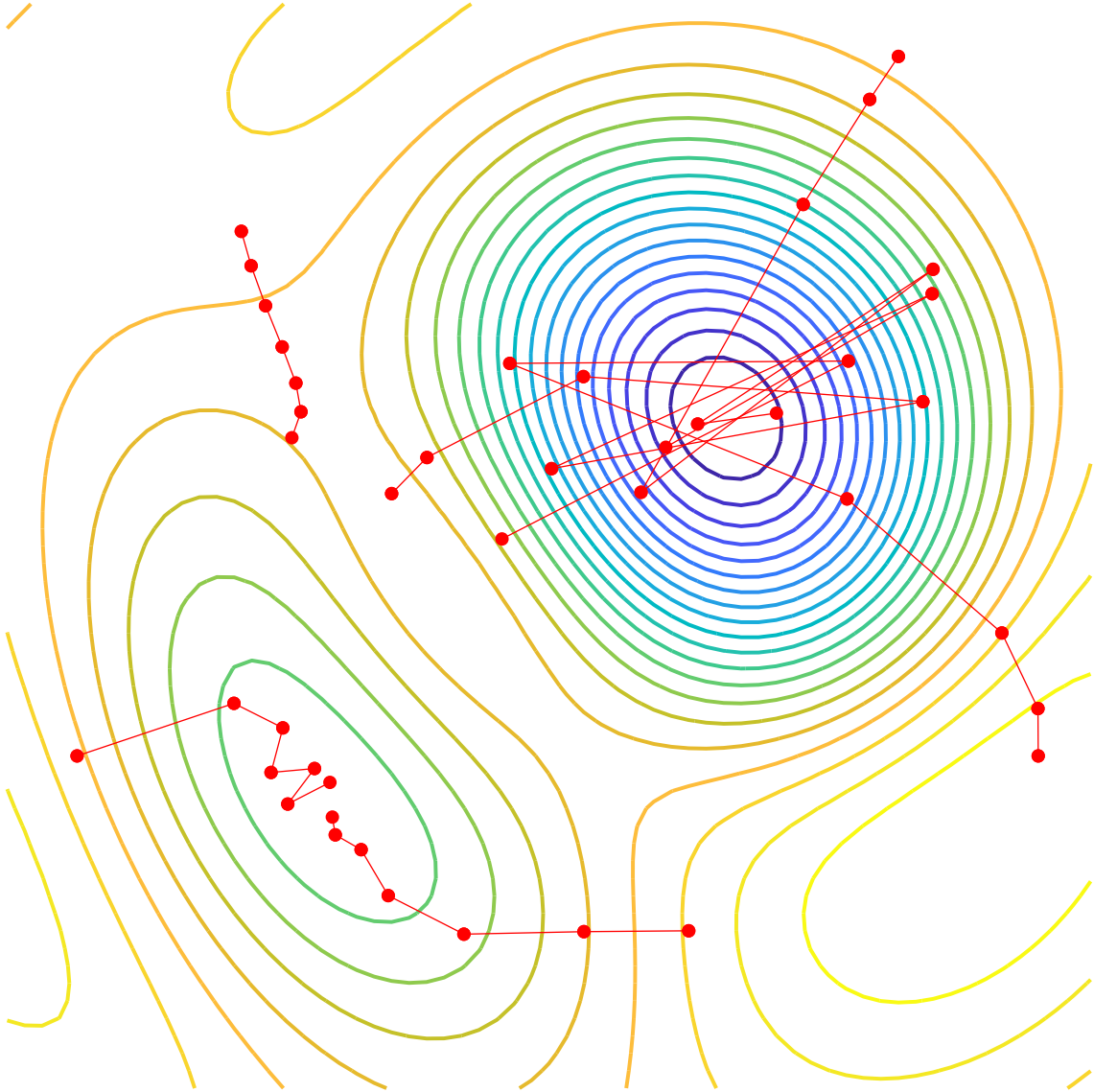
$\epsilon = 0.14$, iteration 4

gradient descent in two dimensions



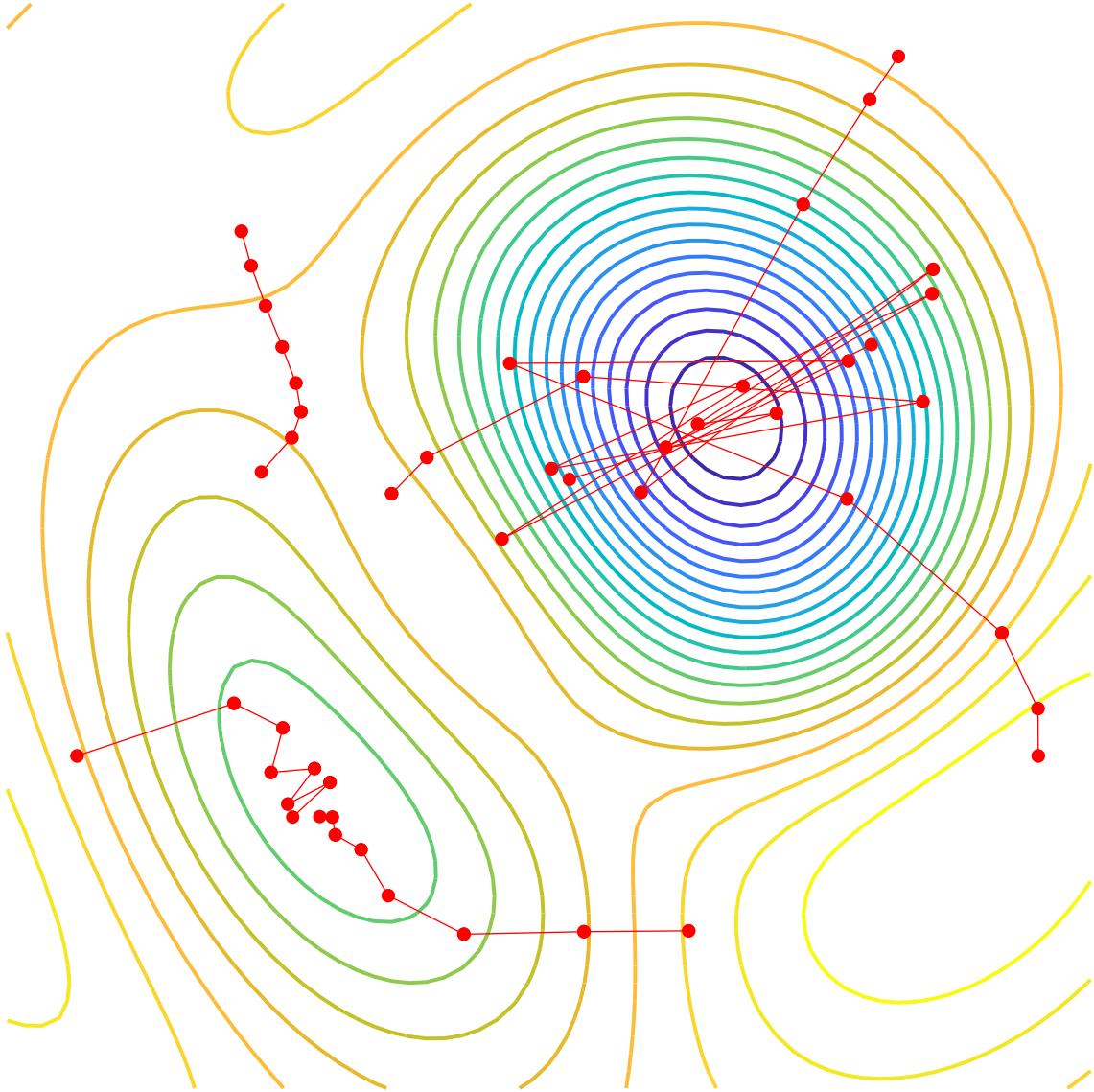
$\epsilon = 0.14$, iteration 5

gradient descent in two dimensions



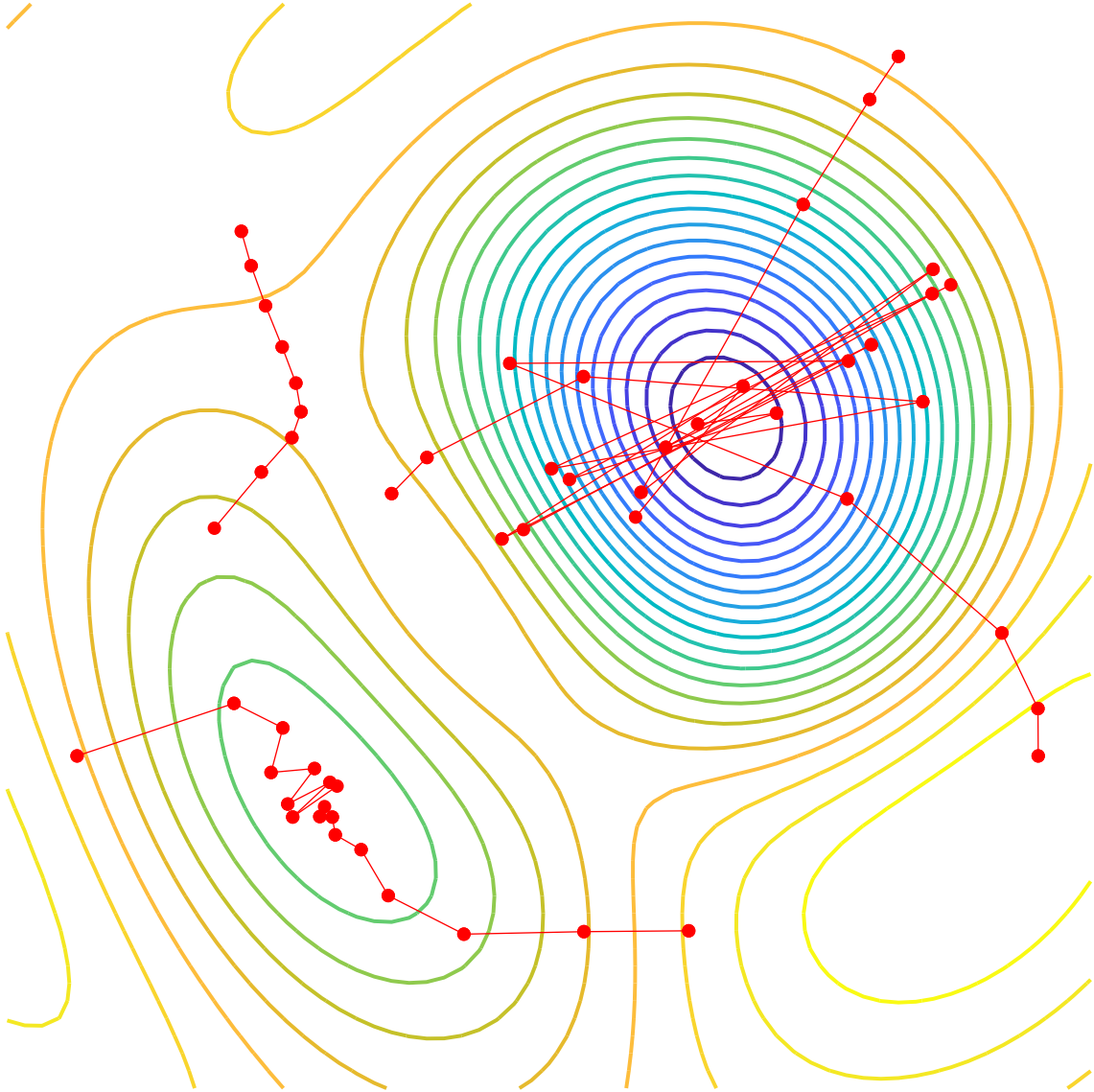
$\epsilon = 0.14$, iteration 6

gradient descent in two dimensions



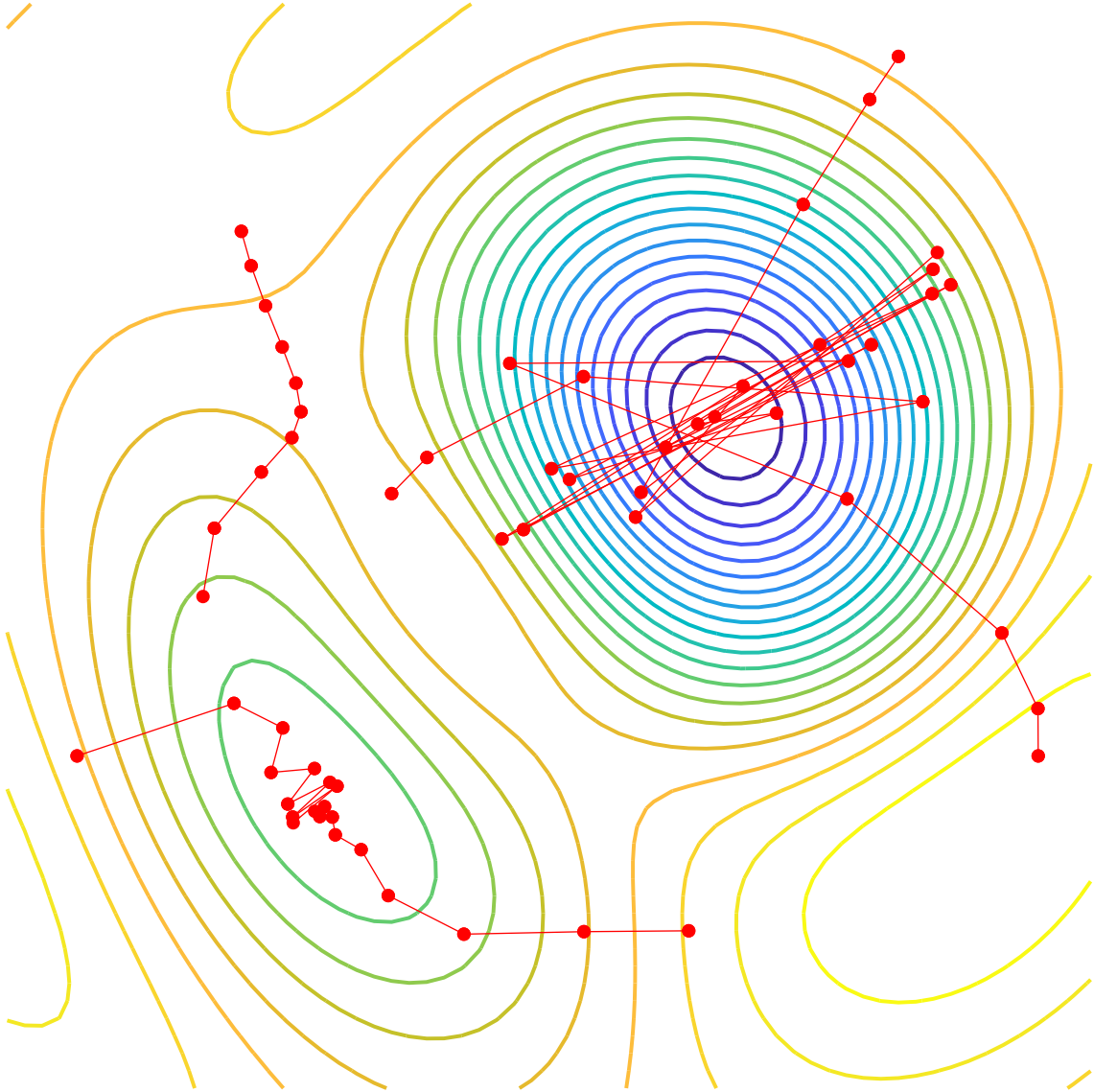
$\epsilon = 0.14$, iteration 7

gradient descent in two dimensions



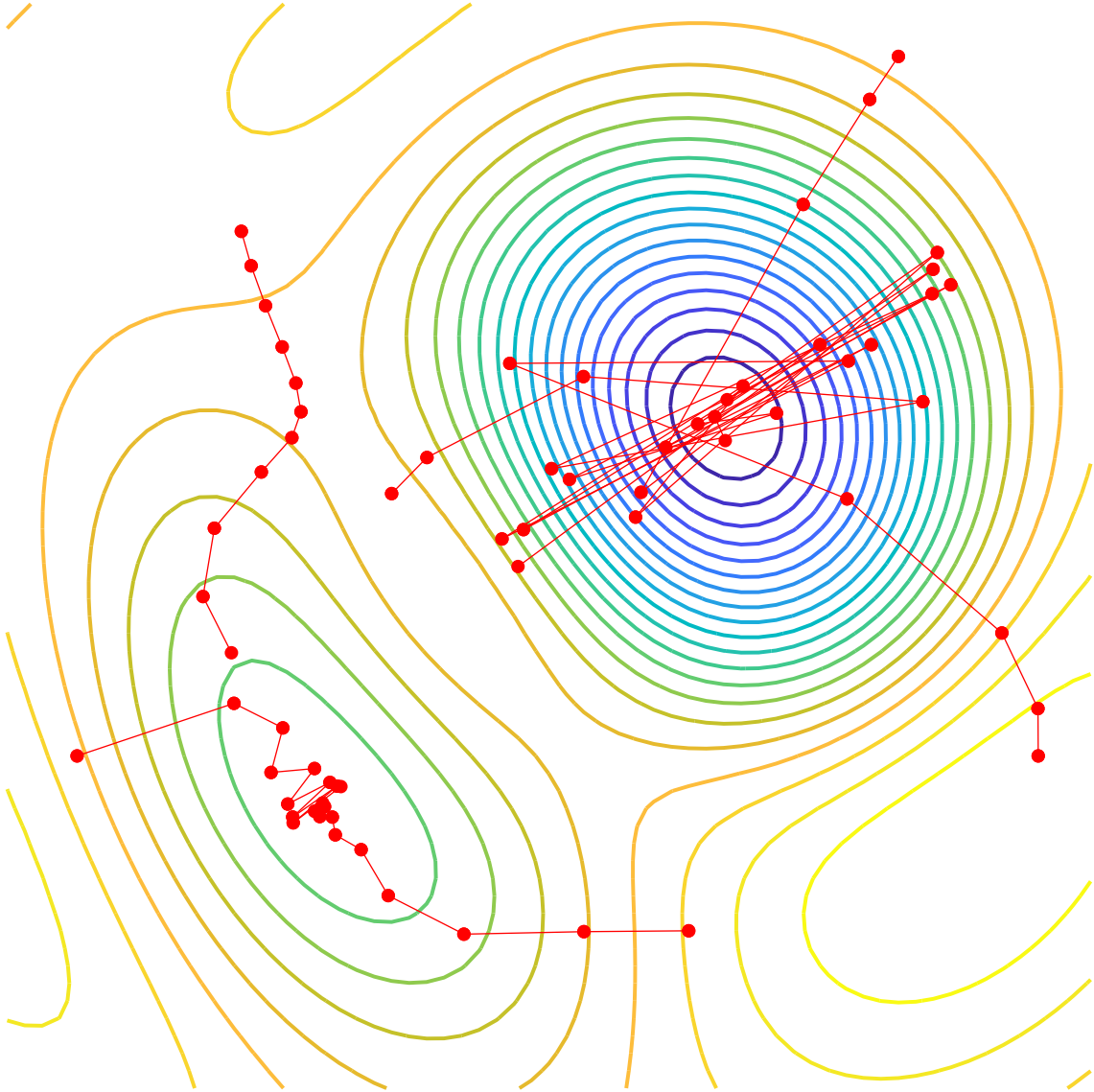
$\epsilon = 0.14$, iteration 8

gradient descent in two dimensions



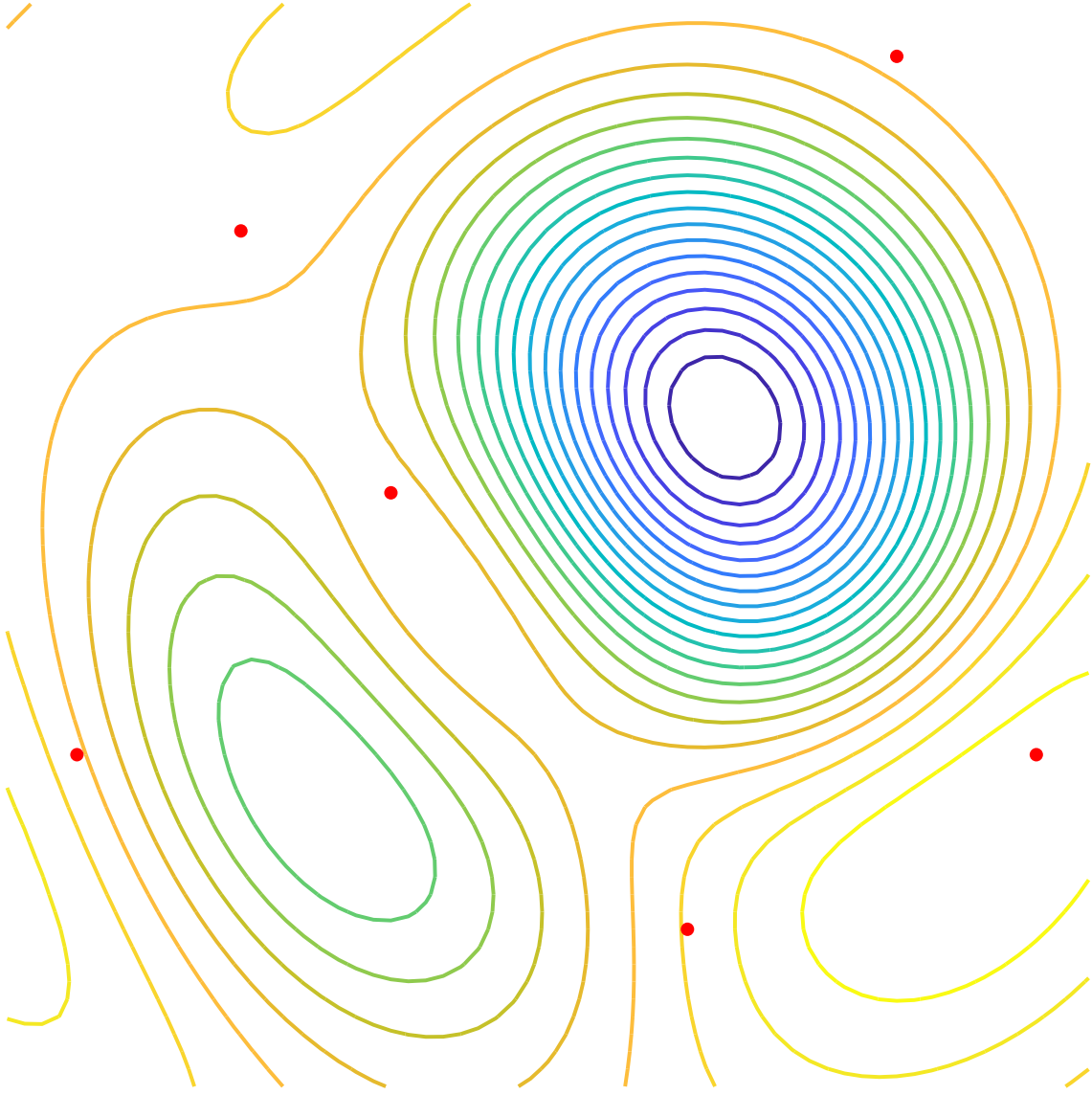
$\epsilon = 0.14$, iteration 9

gradient descent in two dimensions



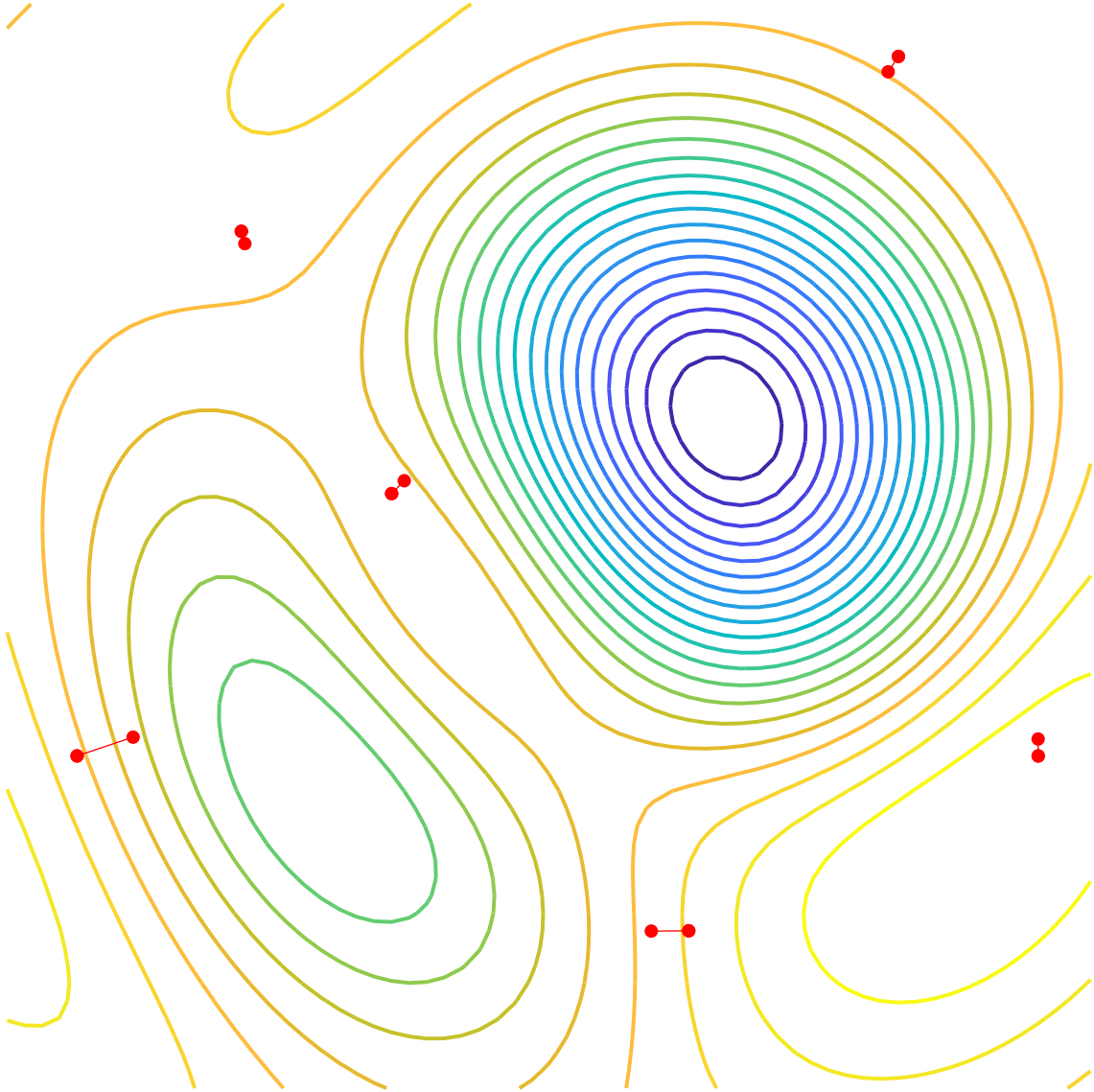
$\epsilon = 0.14$, iteration 10

gradient descent in two dimensions



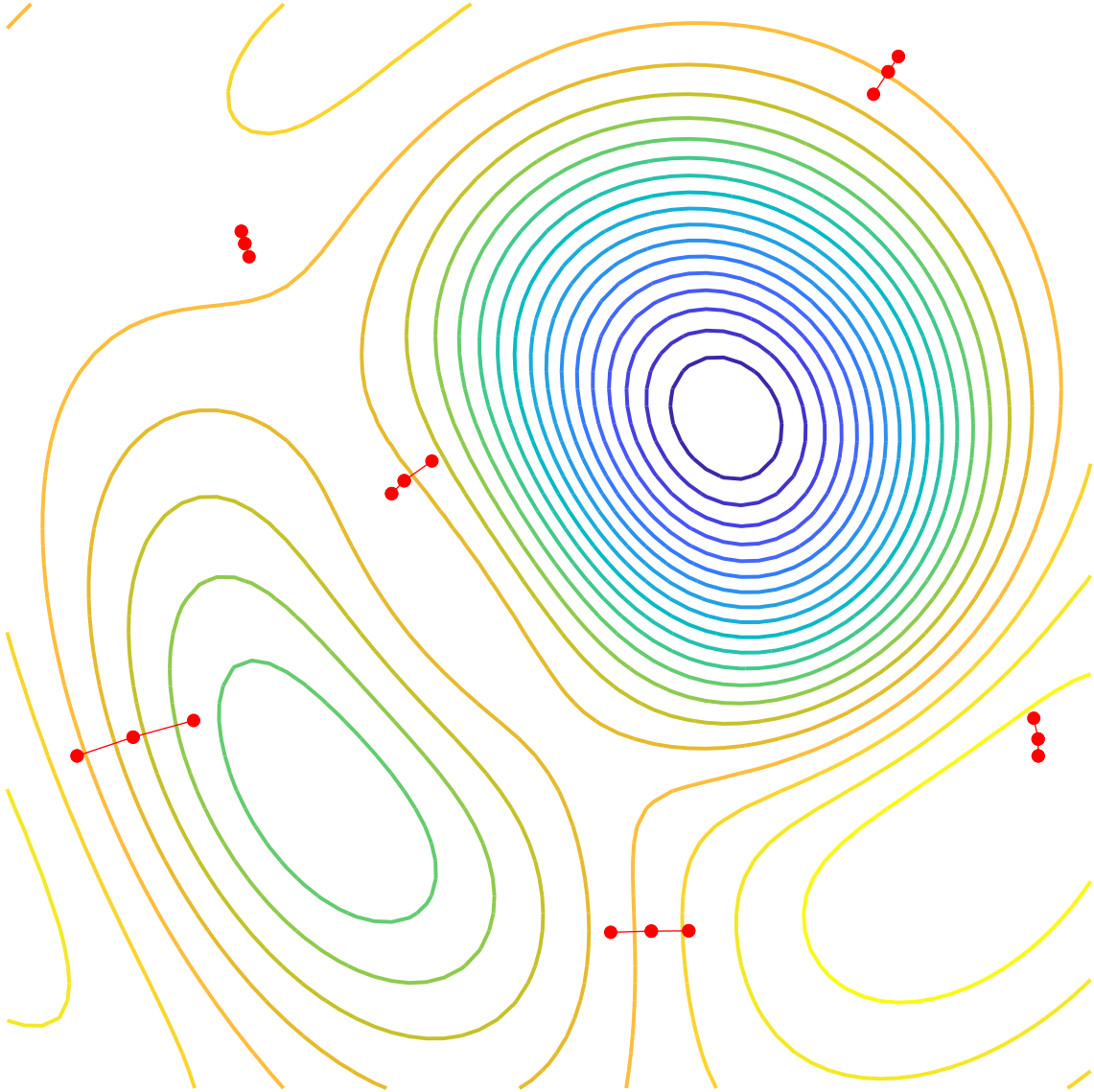
$\epsilon = 0.05$, iteration 0

gradient descent in two dimensions



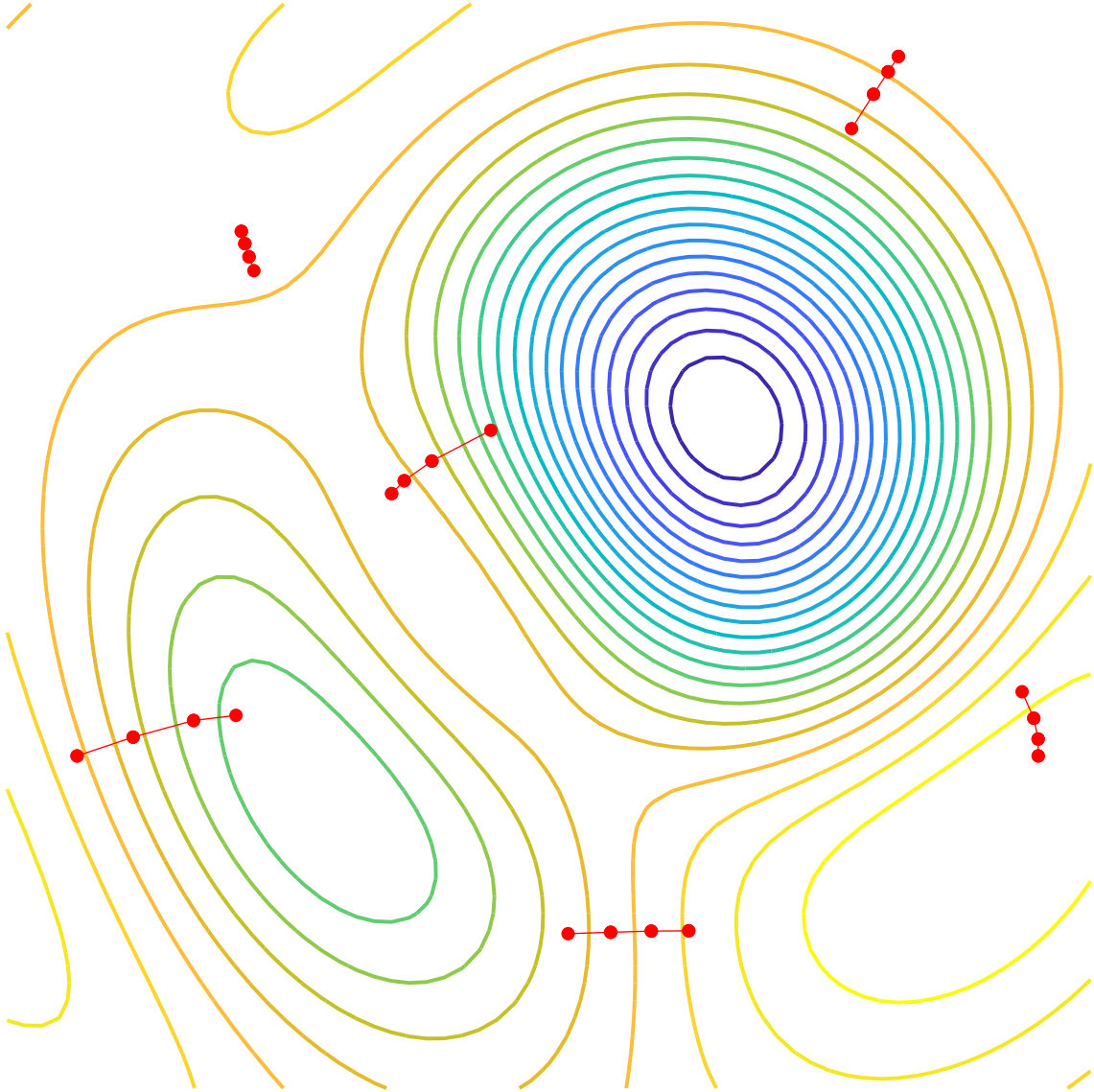
$\epsilon = 0.05$, iteration 1

gradient descent in two dimensions



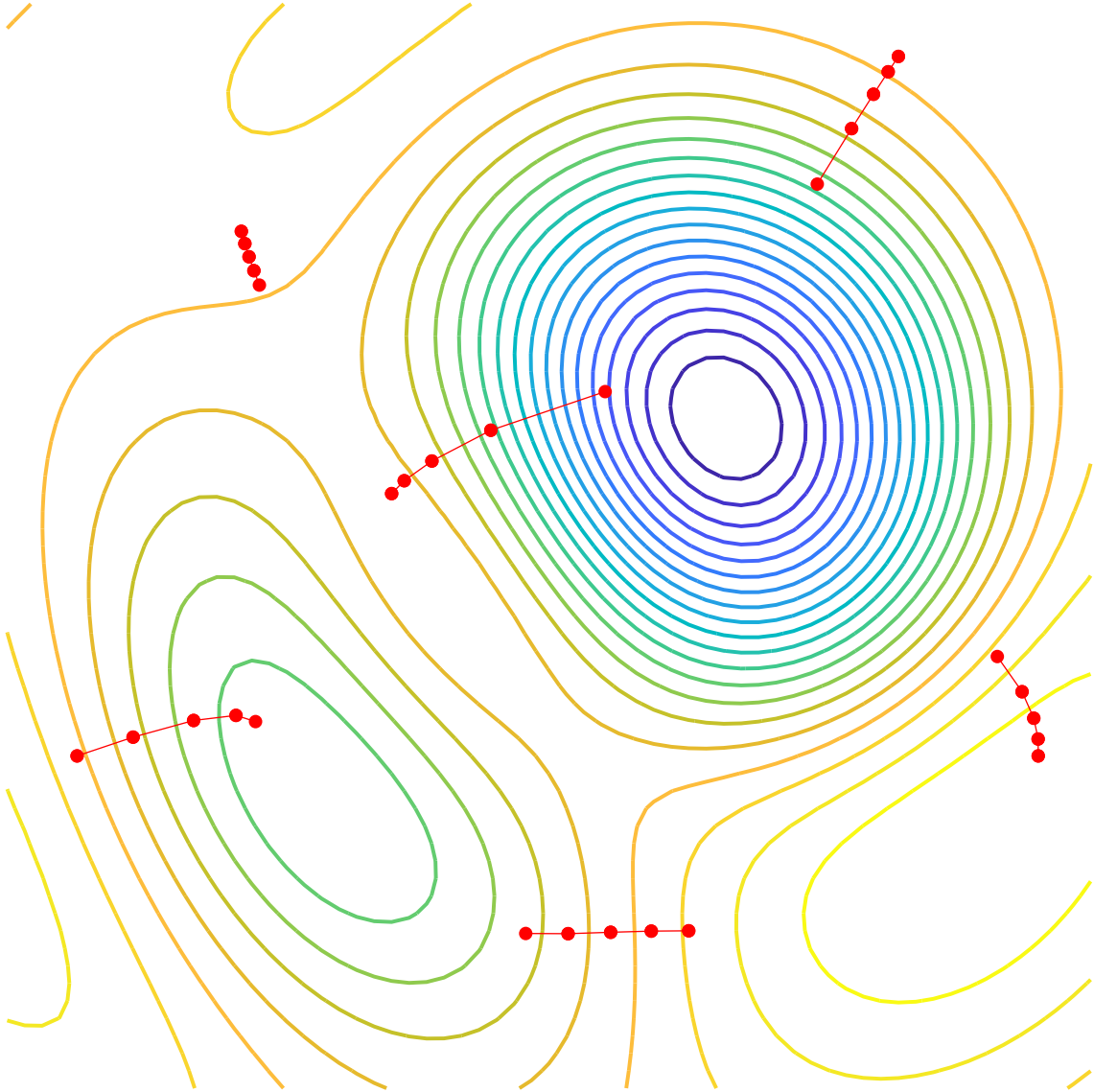
$\epsilon = 0.05$, iteration 2

gradient descent in two dimensions



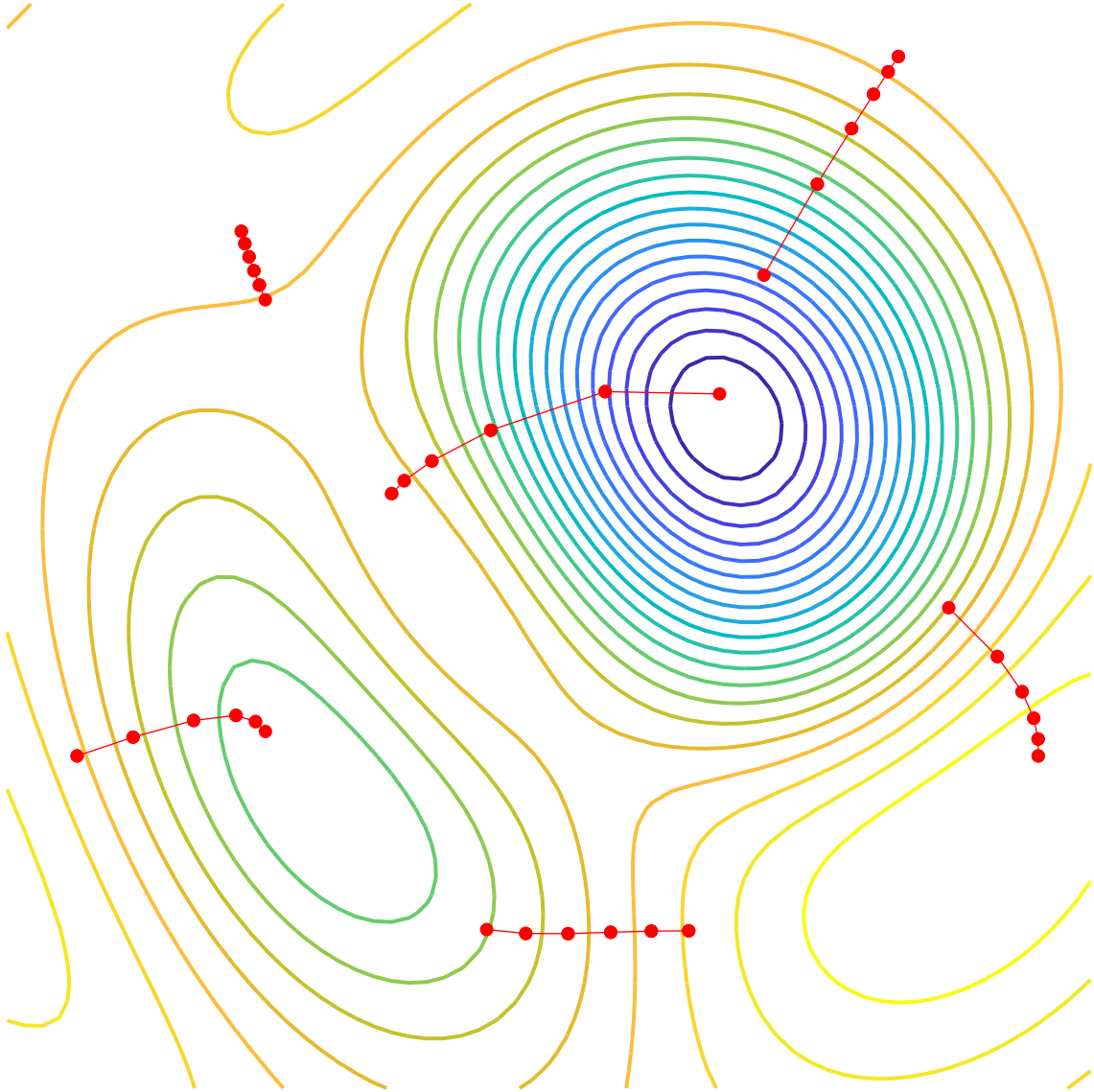
$\epsilon = 0.05$, iteration 3

gradient descent in two dimensions



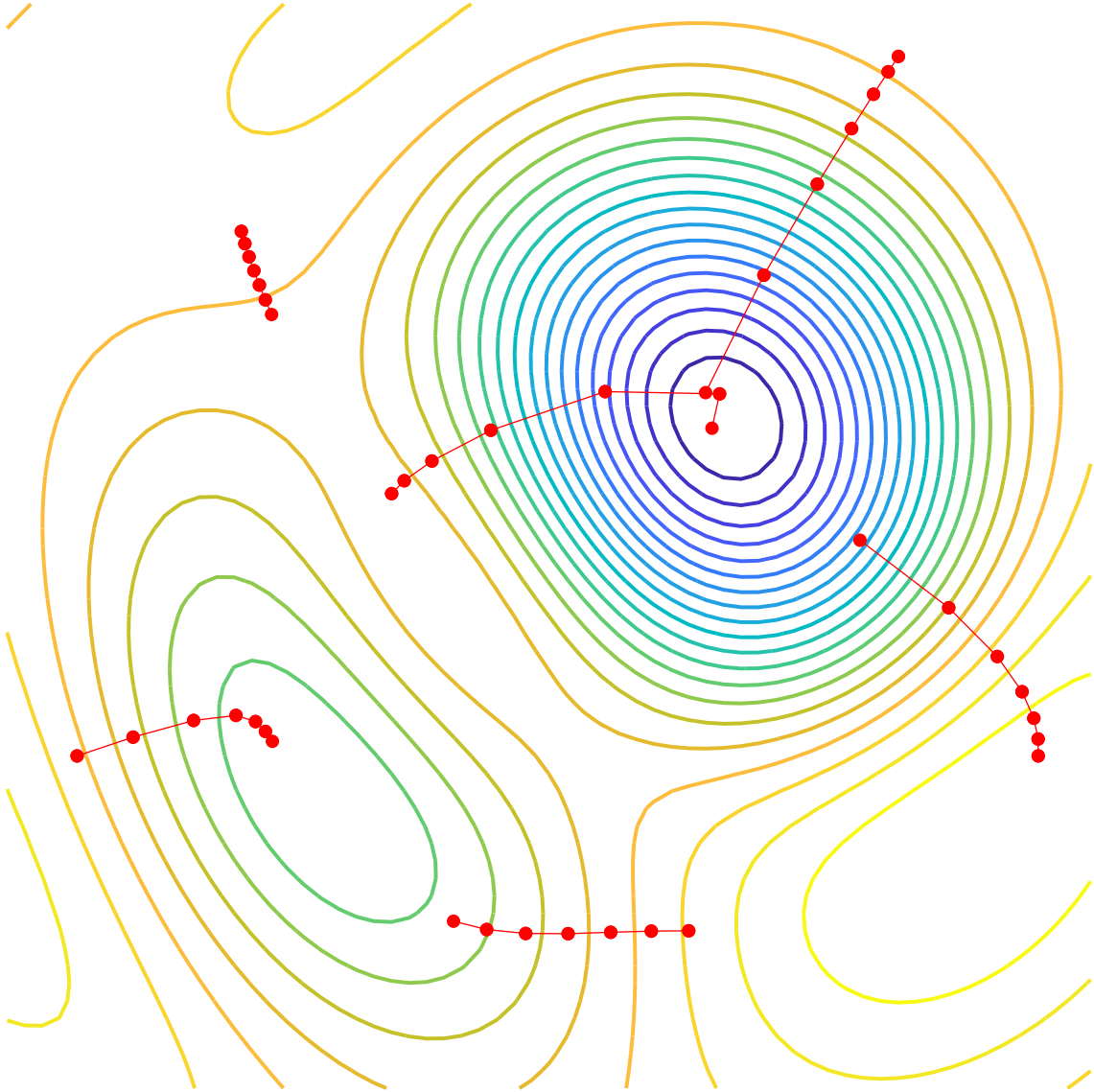
$\epsilon = 0.05$, iteration 4

gradient descent in two dimensions



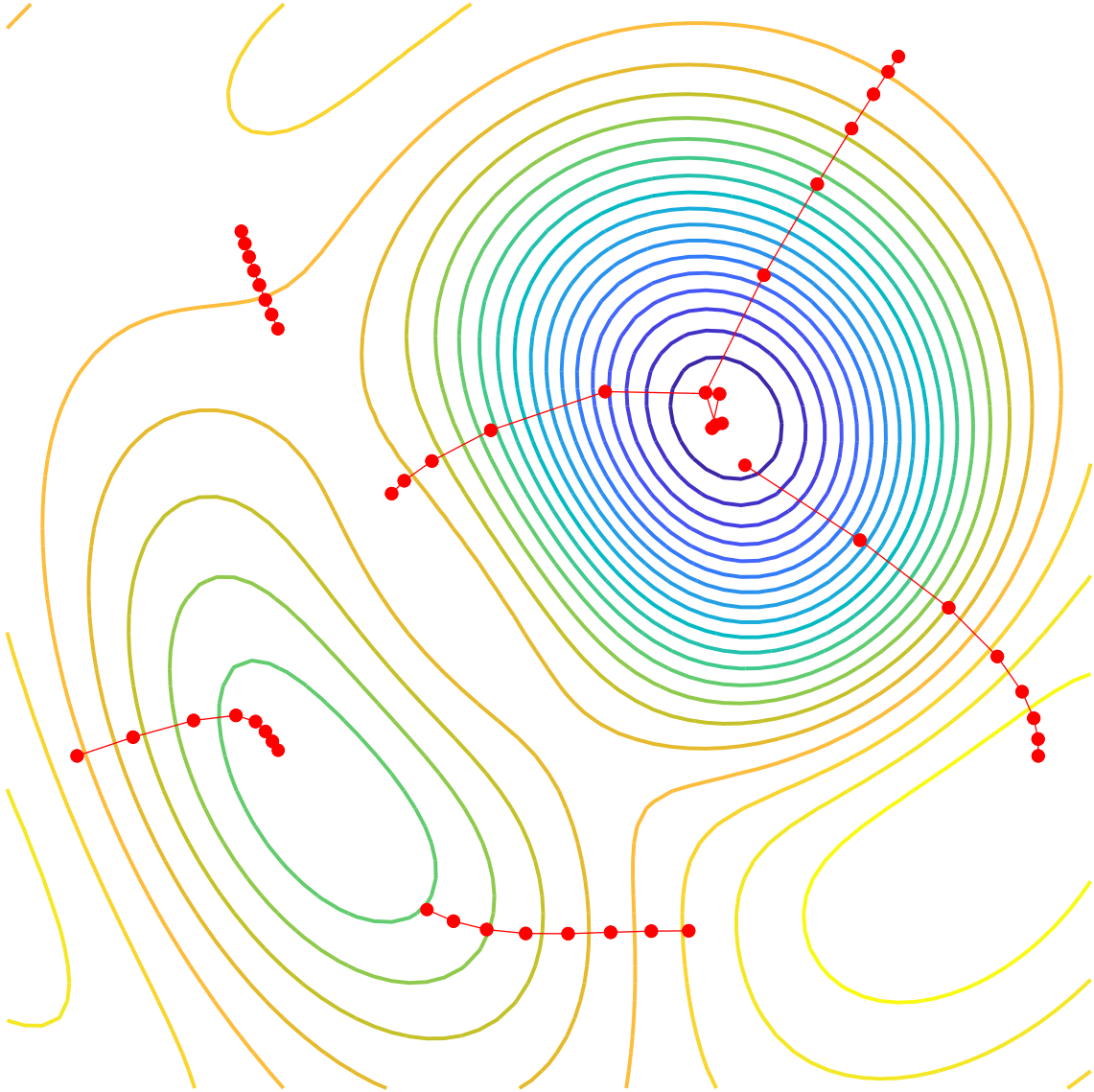
$\epsilon = 0.05$, iteration 5

gradient descent in two dimensions



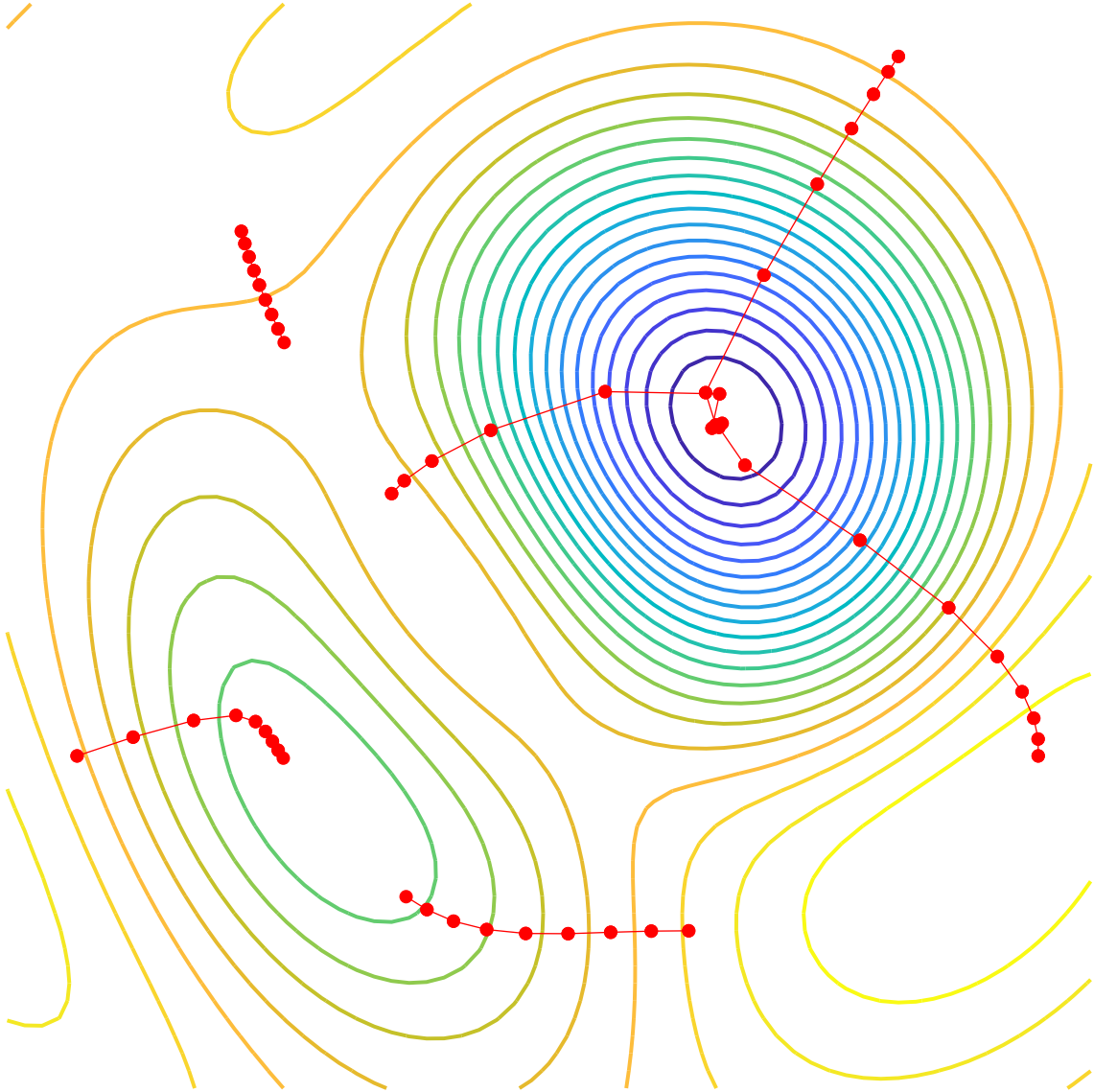
$\epsilon = 0.05$, iteration 6

gradient descent in two dimensions



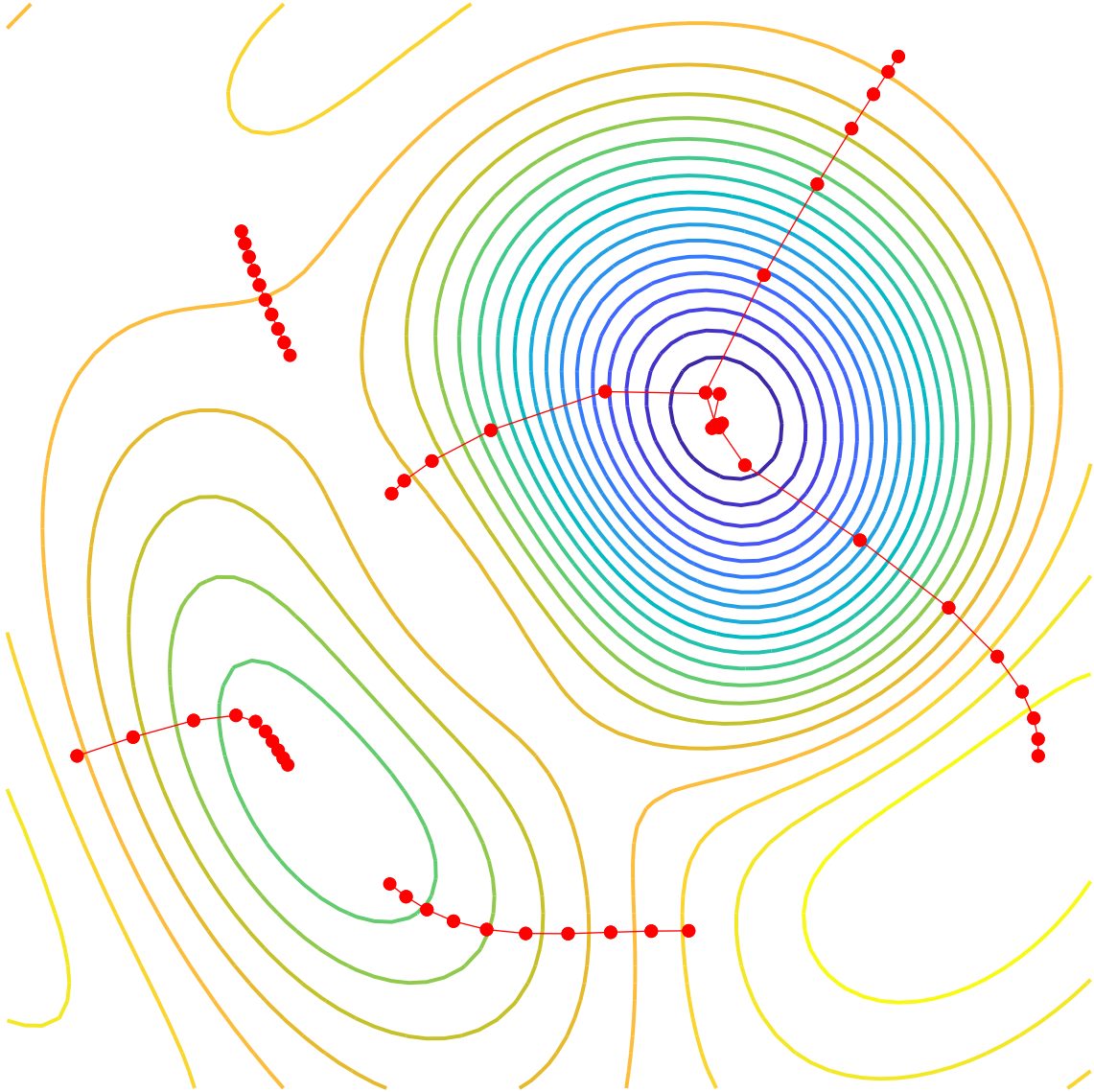
$\epsilon = 0.05$, iteration 7

gradient descent in two dimensions



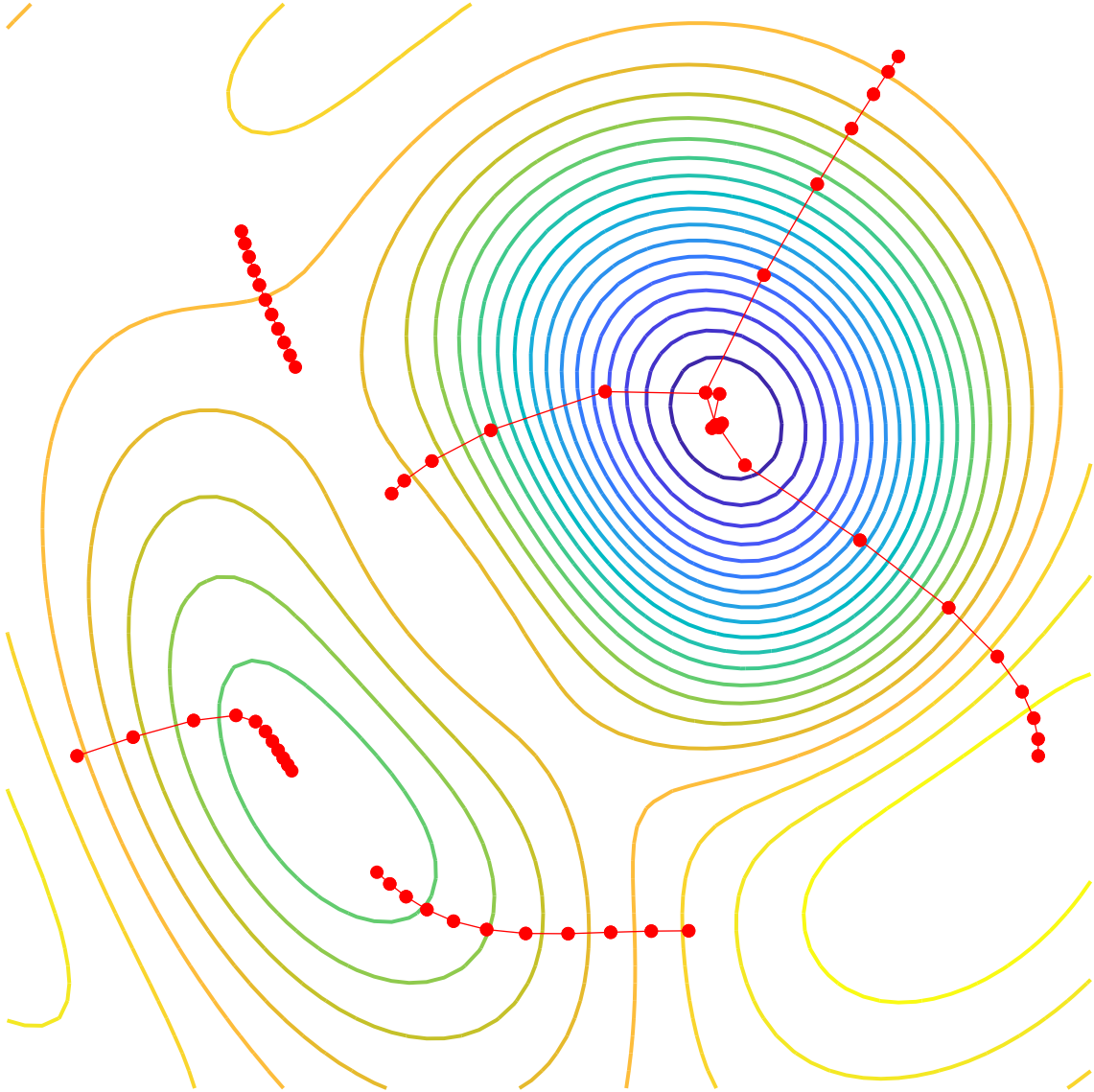
$\epsilon = 0.05$, iteration 8

gradient descent in two dimensions



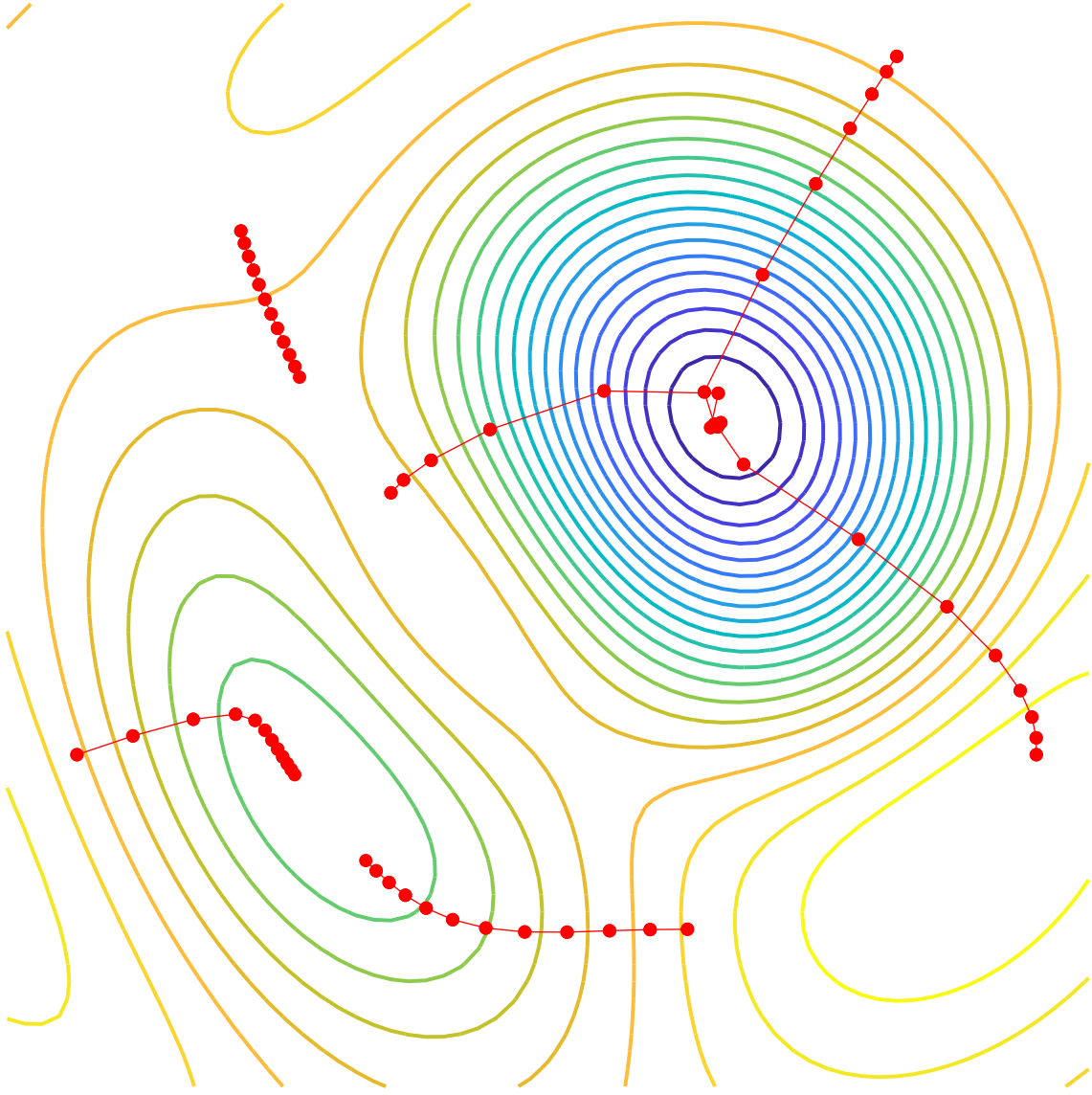
$\epsilon = 0.05$, iteration 9

gradient descent in two dimensions



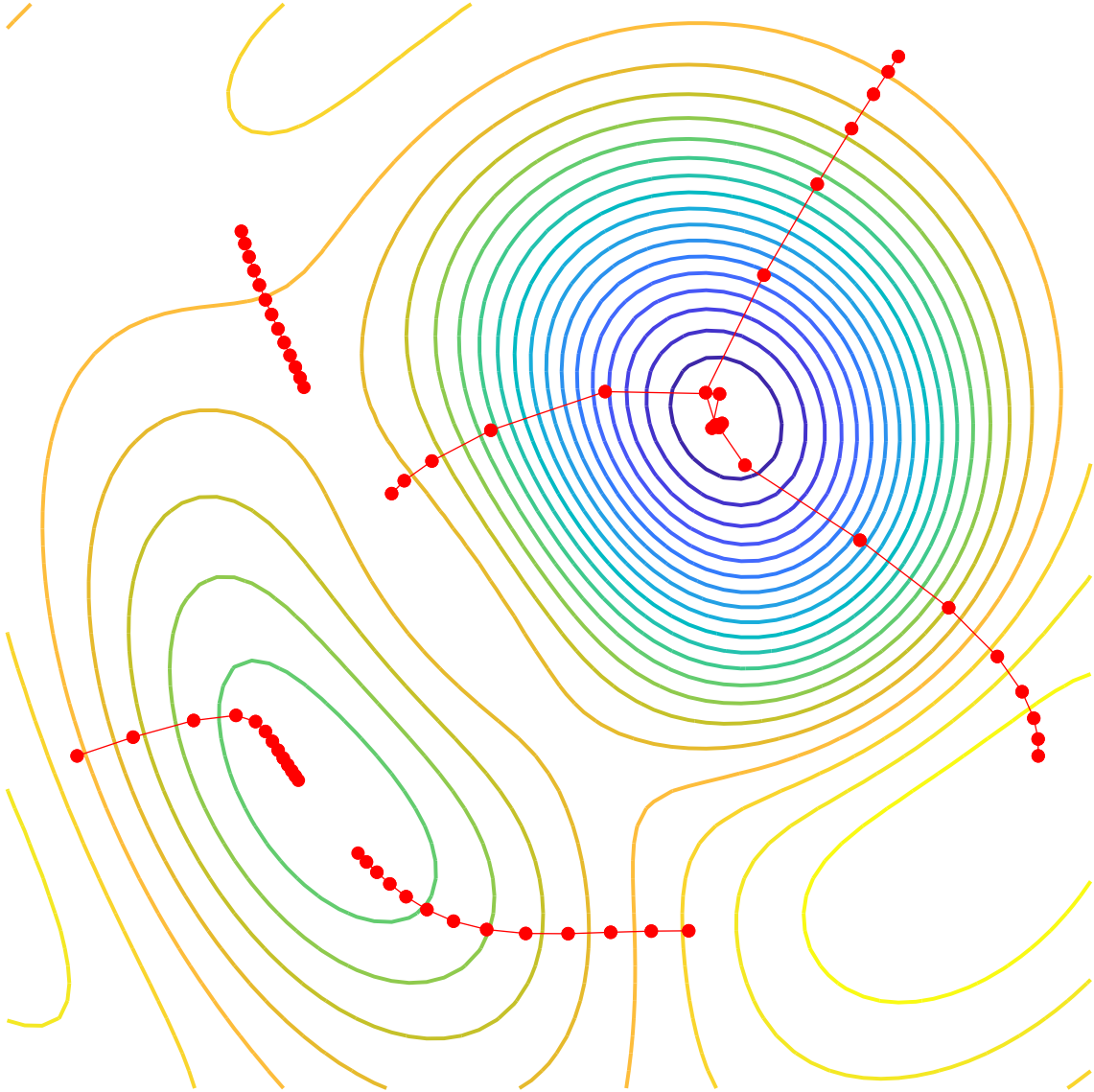
$\epsilon = 0.05$, iteration 10

gradient descent in two dimensions



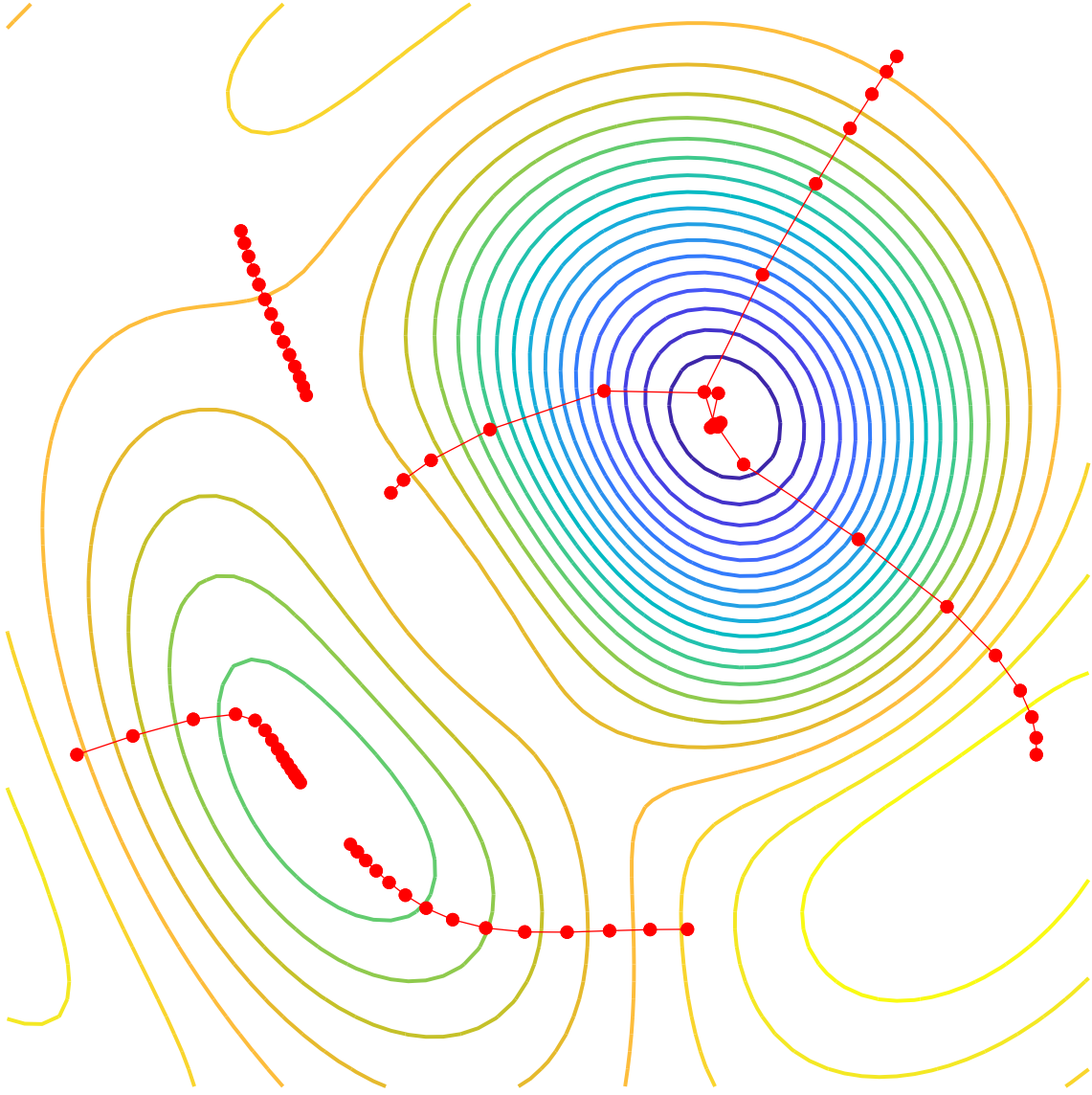
$\epsilon = 0.05$, iteration 11

gradient descent in two dimensions



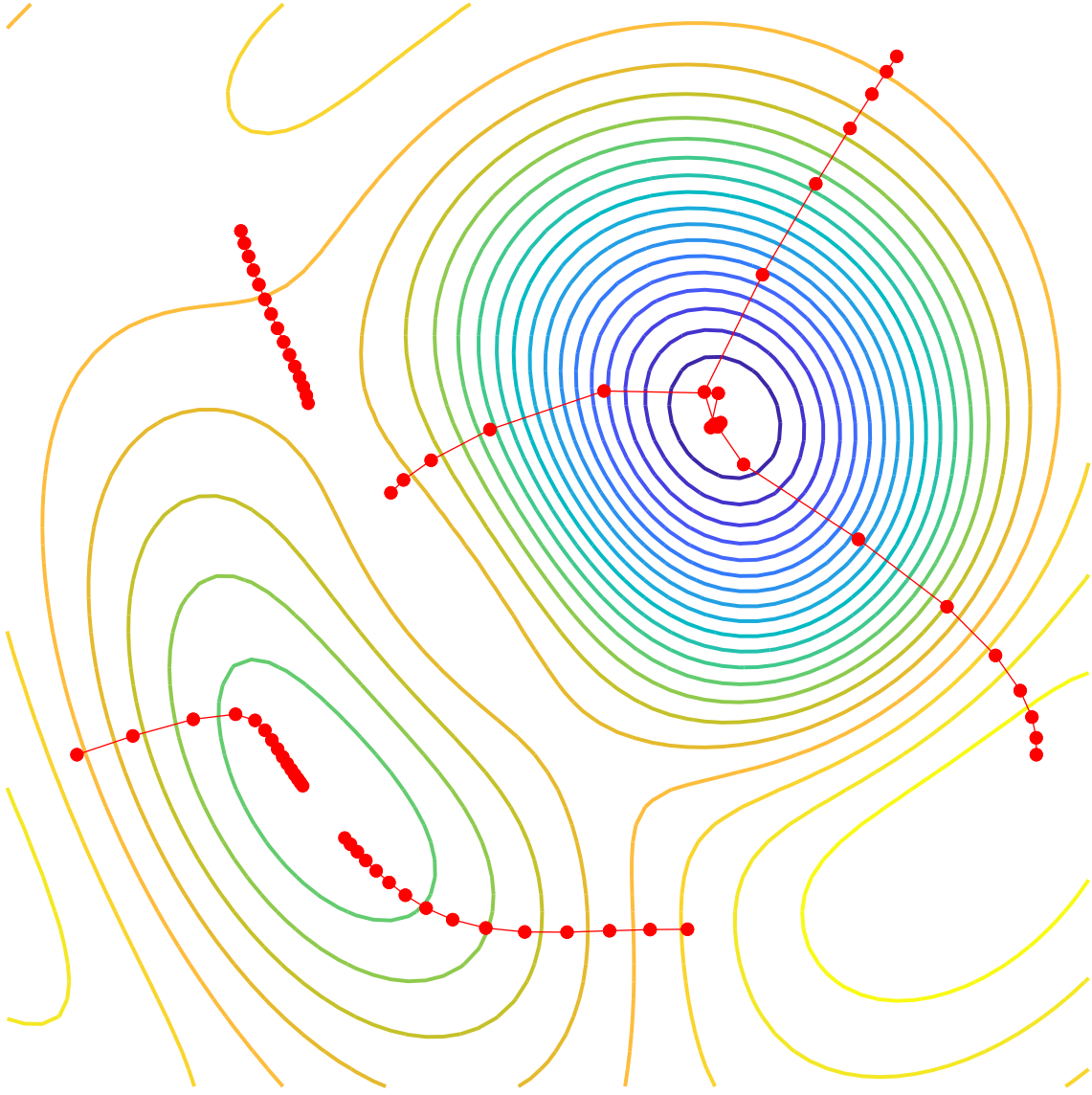
$\epsilon = 0.05$, iteration 12

gradient descent in two dimensions



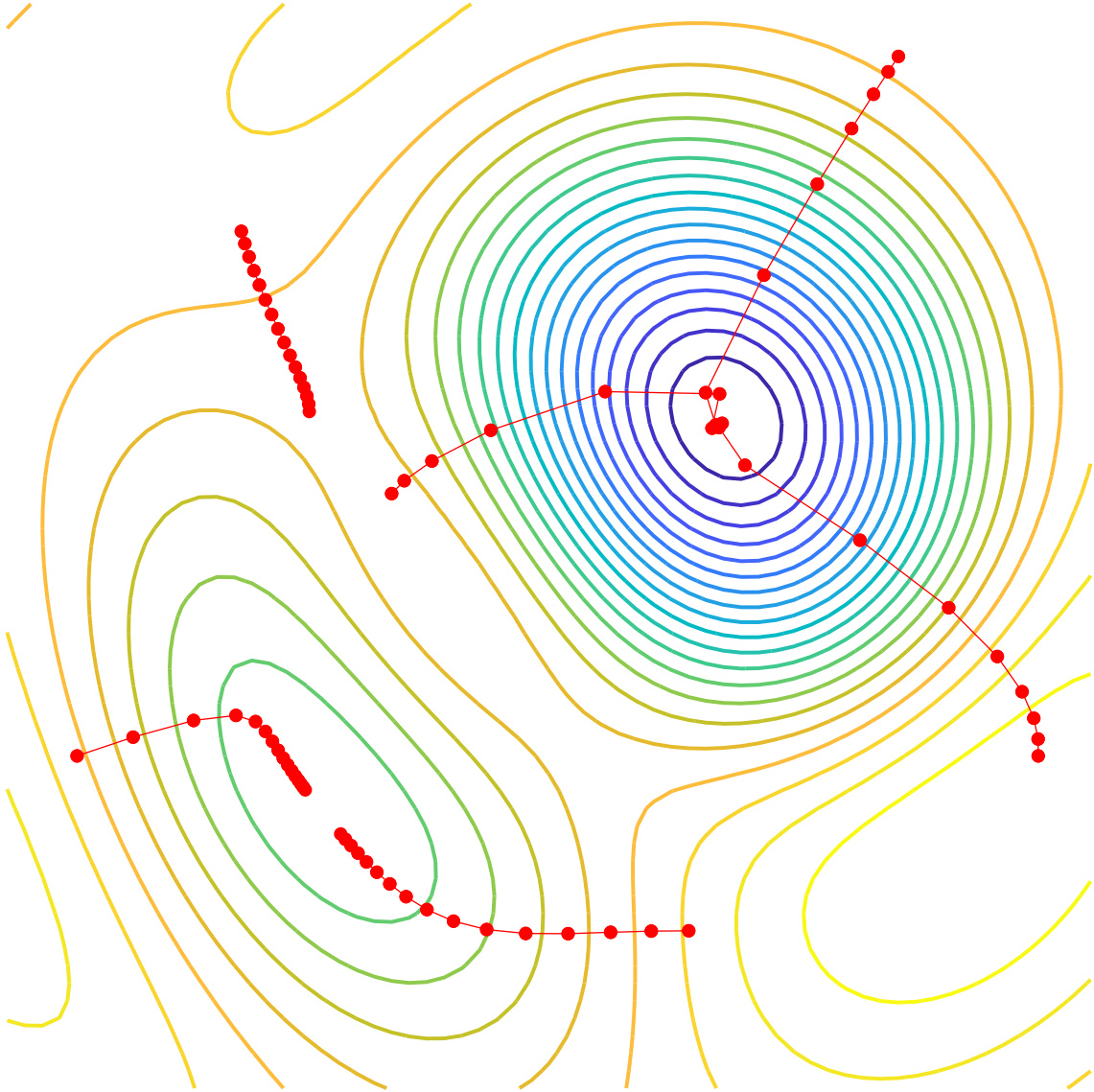
$\epsilon = 0.05$, iteration 13

gradient descent in two dimensions



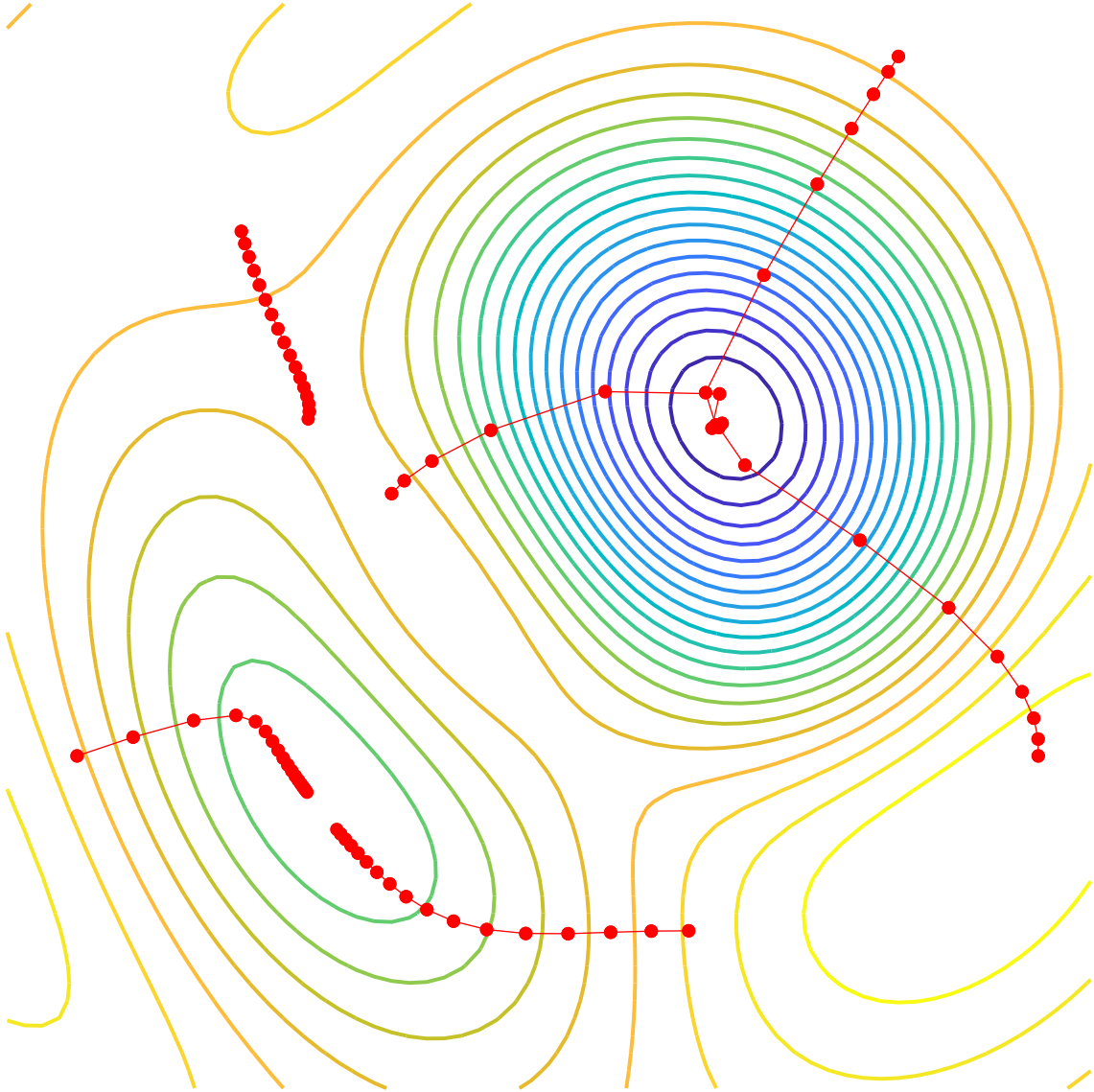
$\epsilon = 0.05$, iteration 14

gradient descent in two dimensions



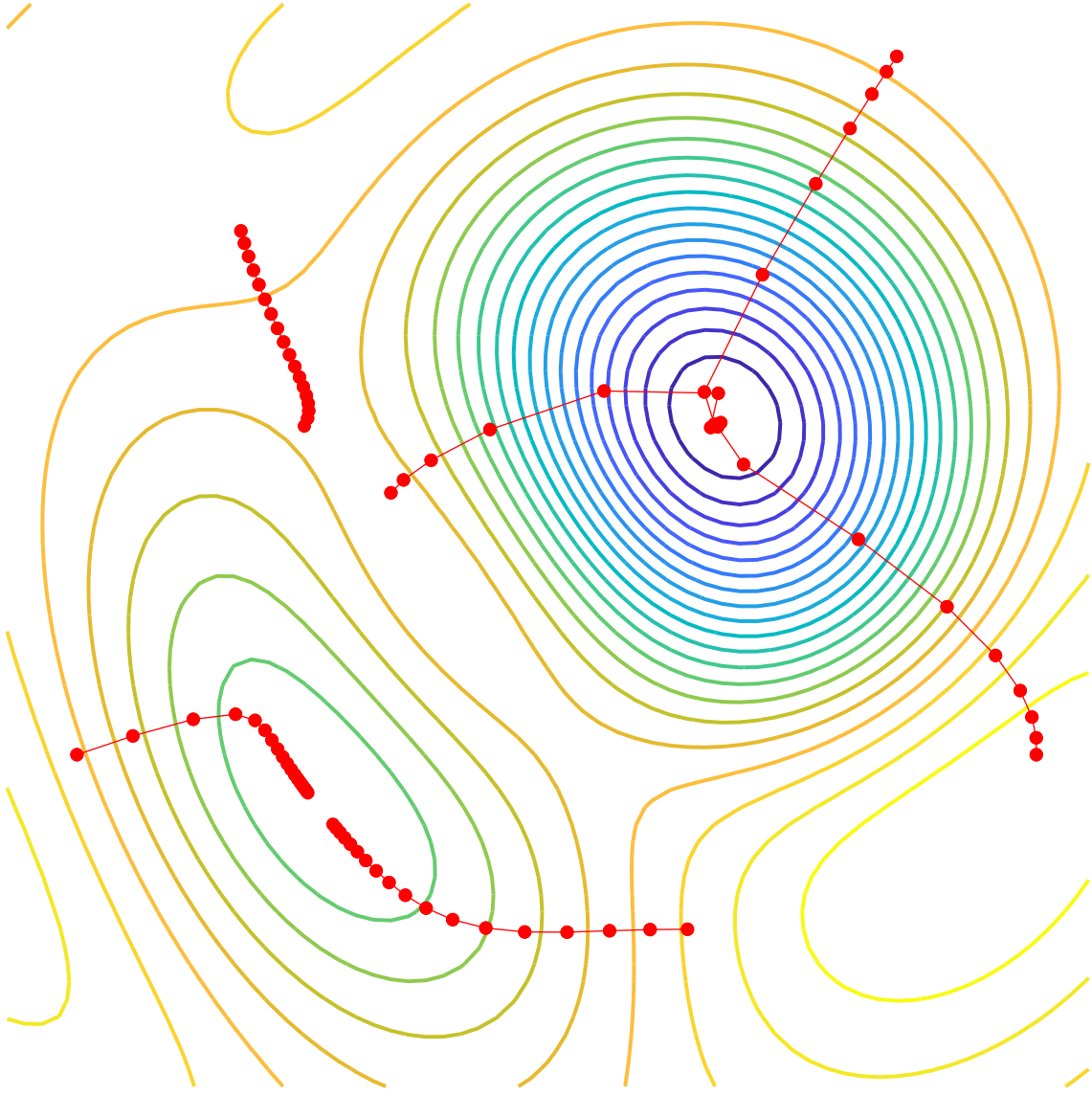
$\epsilon = 0.05$, iteration 15

gradient descent in two dimensions



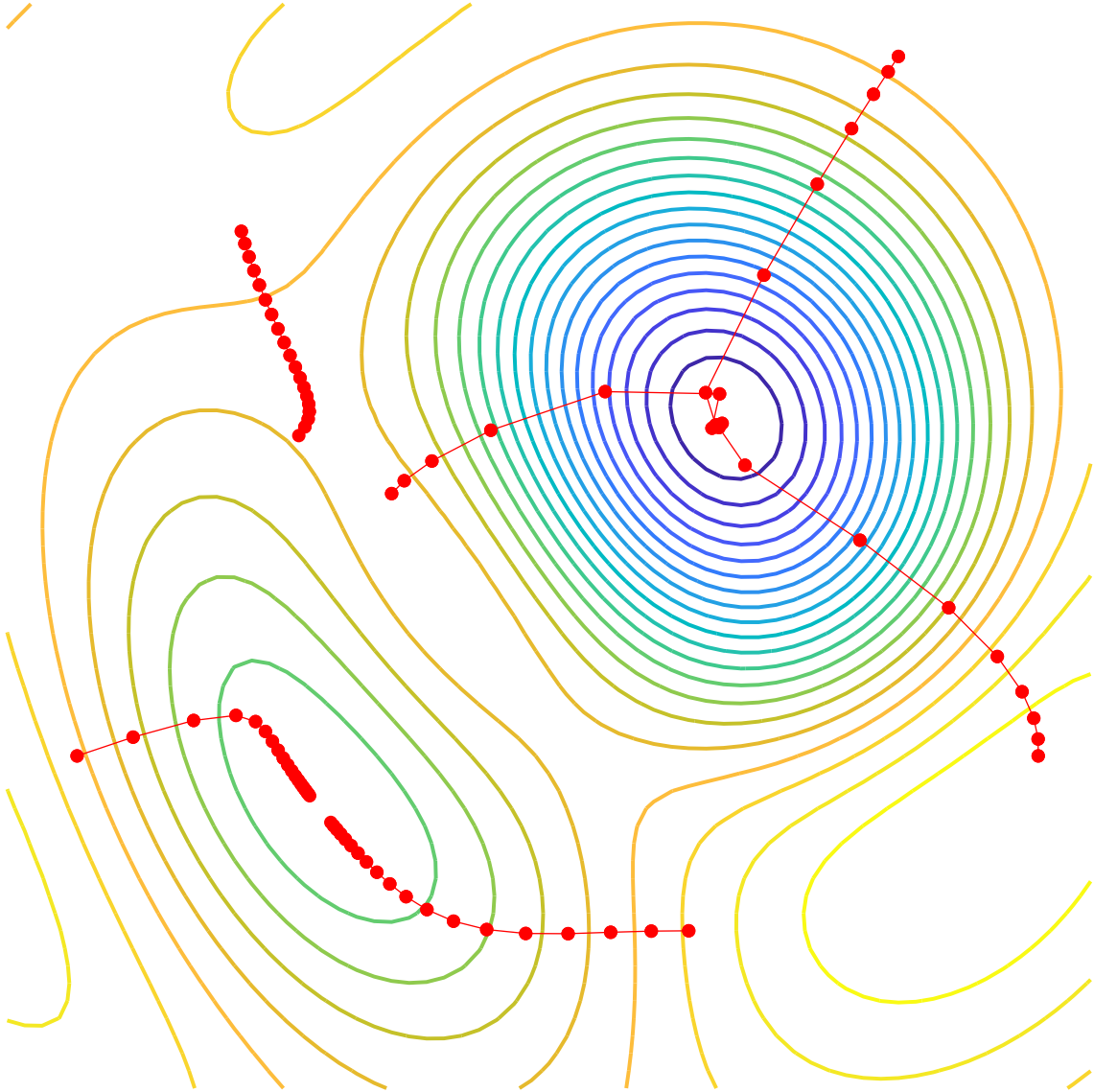
$\epsilon = 0.05$, iteration 16

gradient descent in two dimensions



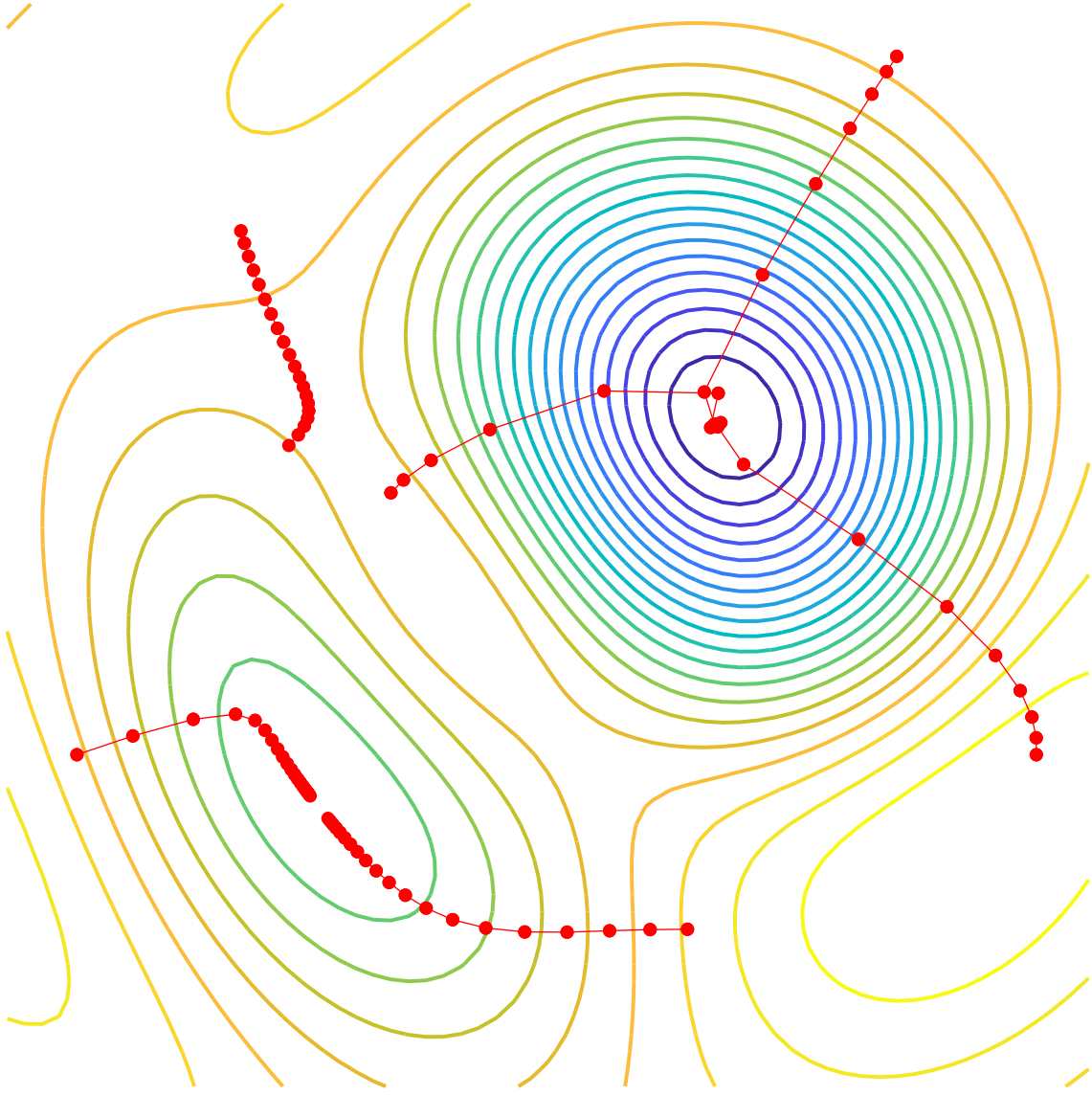
$\epsilon = 0.05$, iteration 17

gradient descent in two dimensions



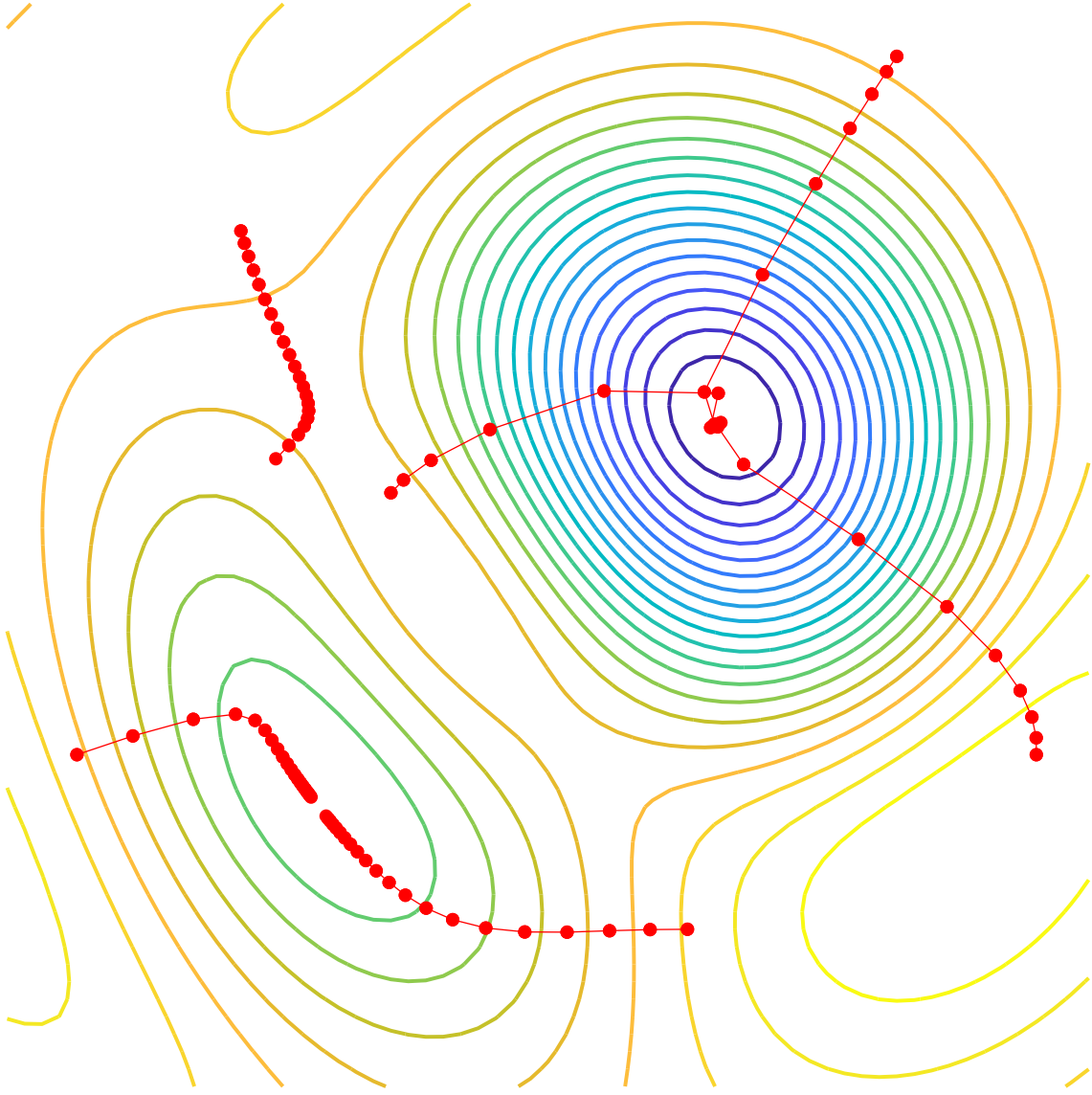
$\epsilon = 0.05$, iteration 18

gradient descent in two dimensions



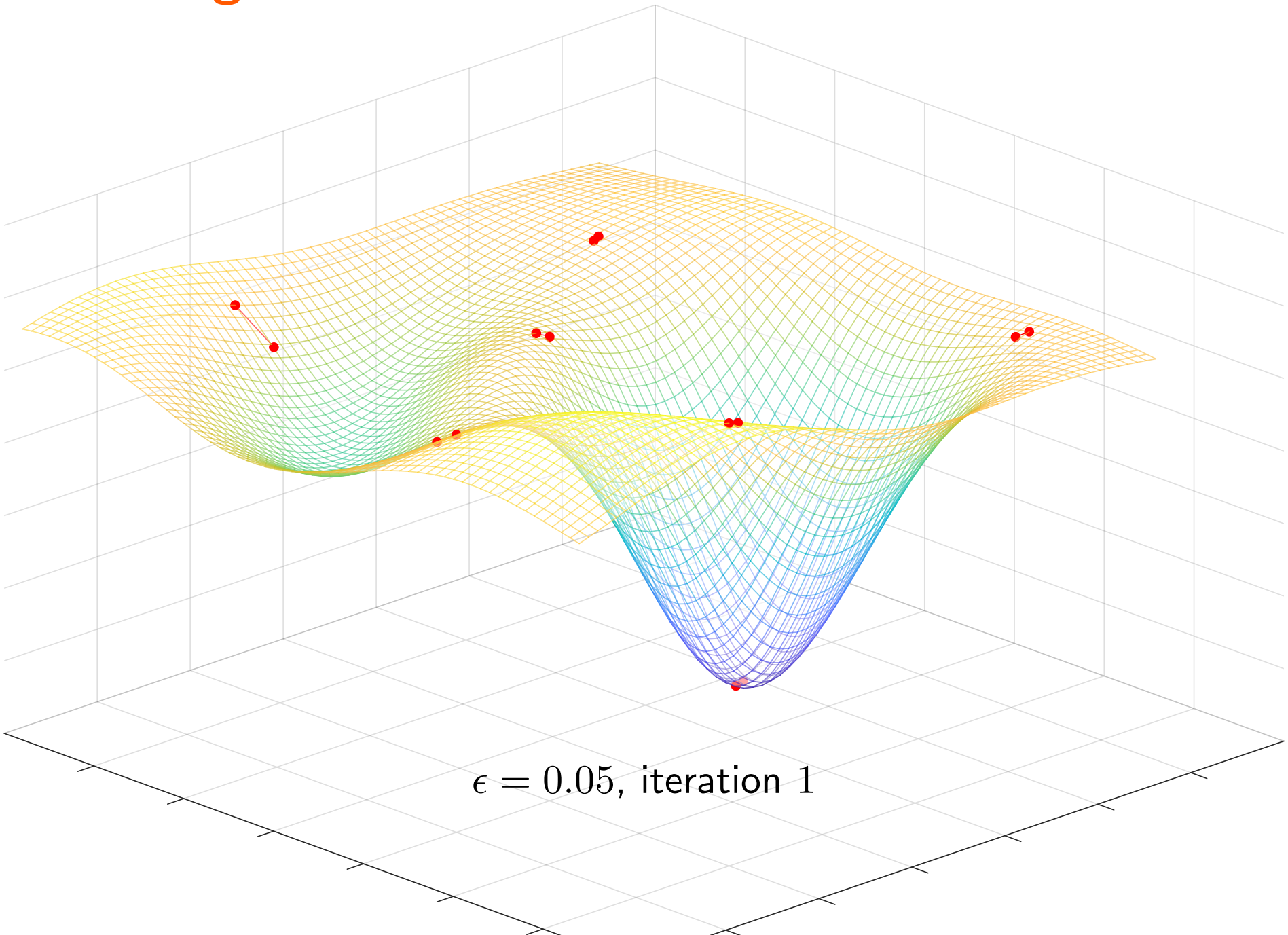
$\epsilon = 0.05$, iteration 19

gradient descent in two dimensions



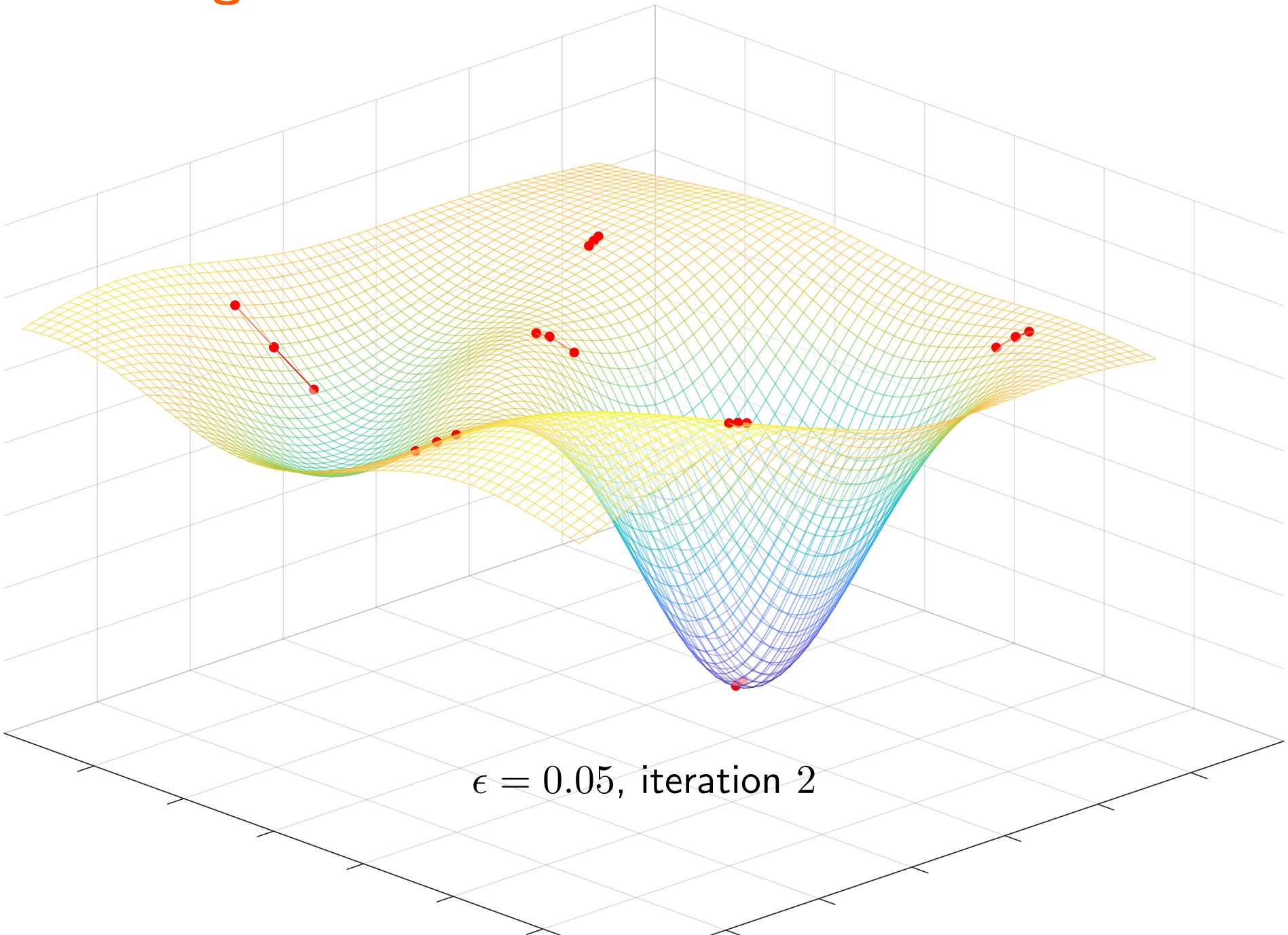
$\epsilon = 0.05$, iteration 20

gradient descent in two dimensions



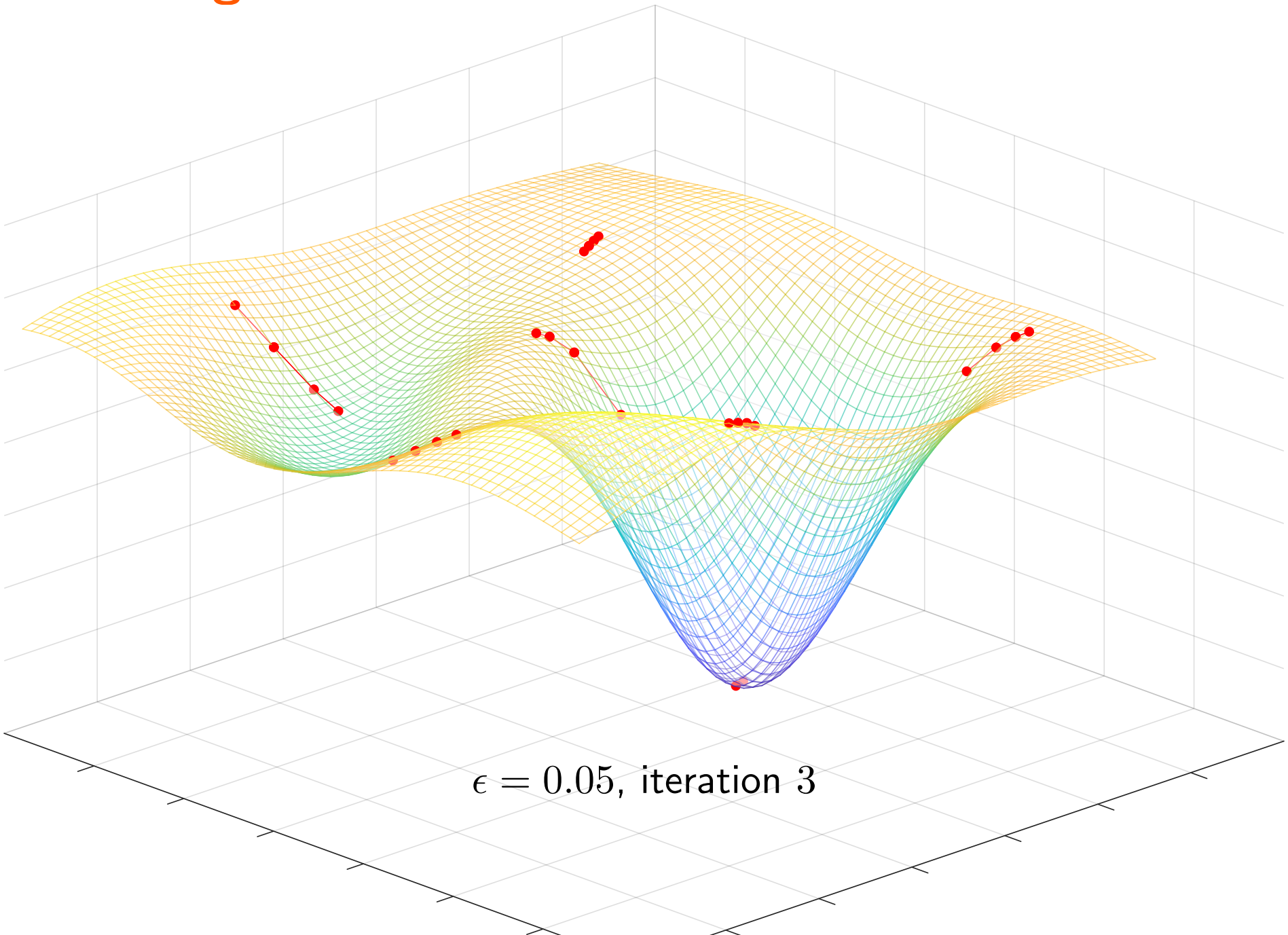
$\epsilon = 0.05$, iteration 1

gradient descent in two dimensions

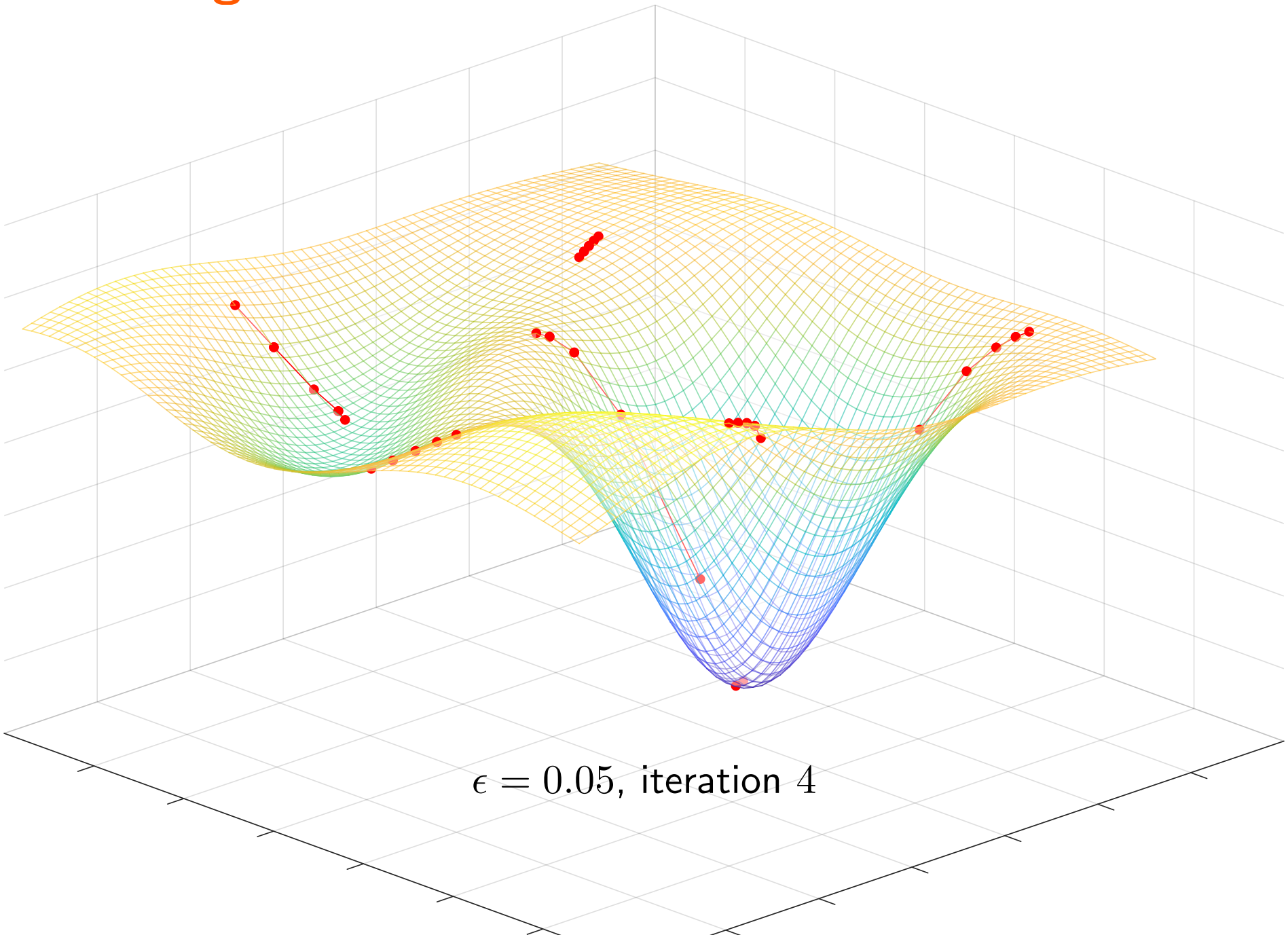


$\epsilon = 0.05$, iteration 2

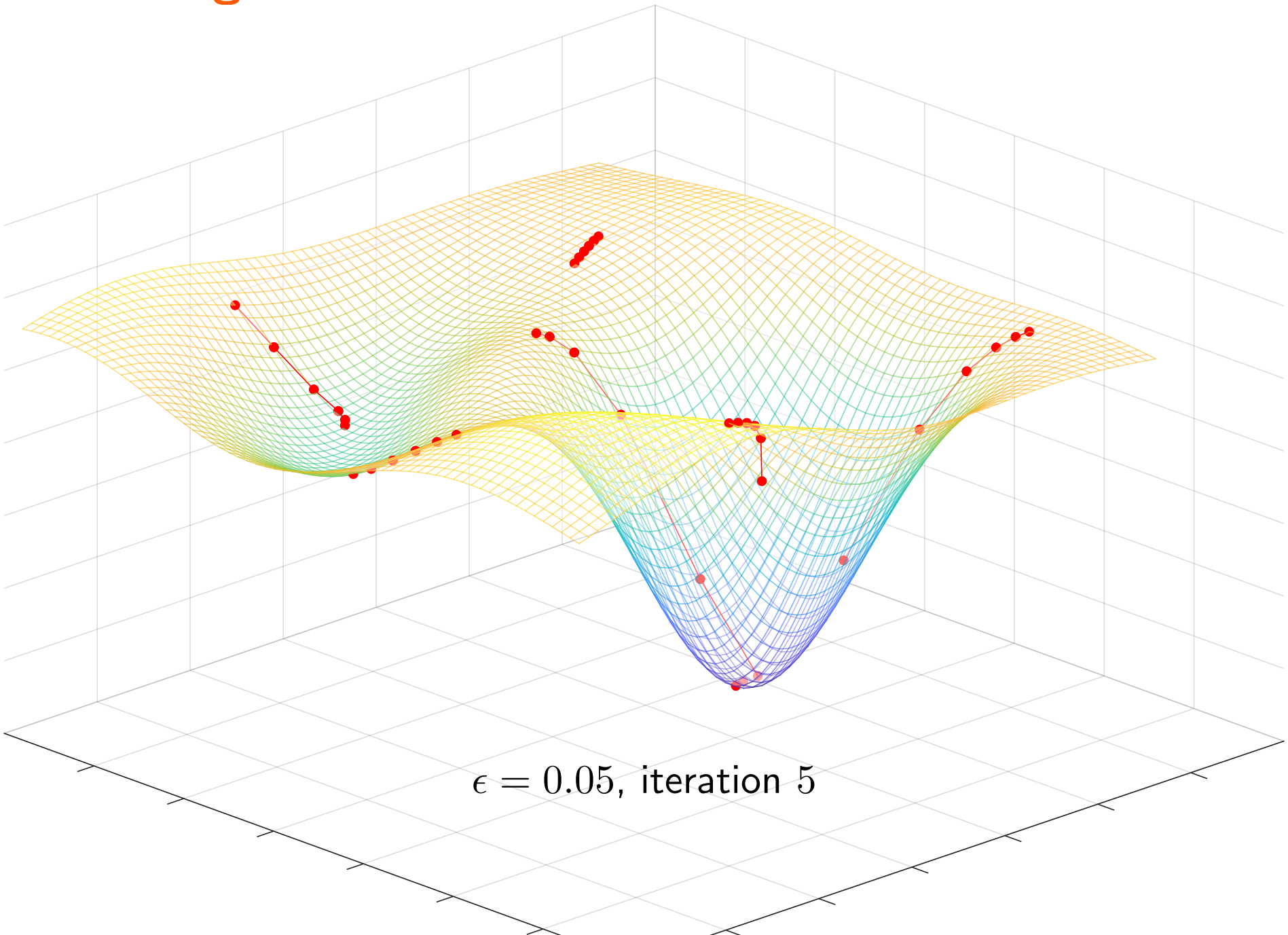
gradient descent in two dimensions



gradient descent in two dimensions

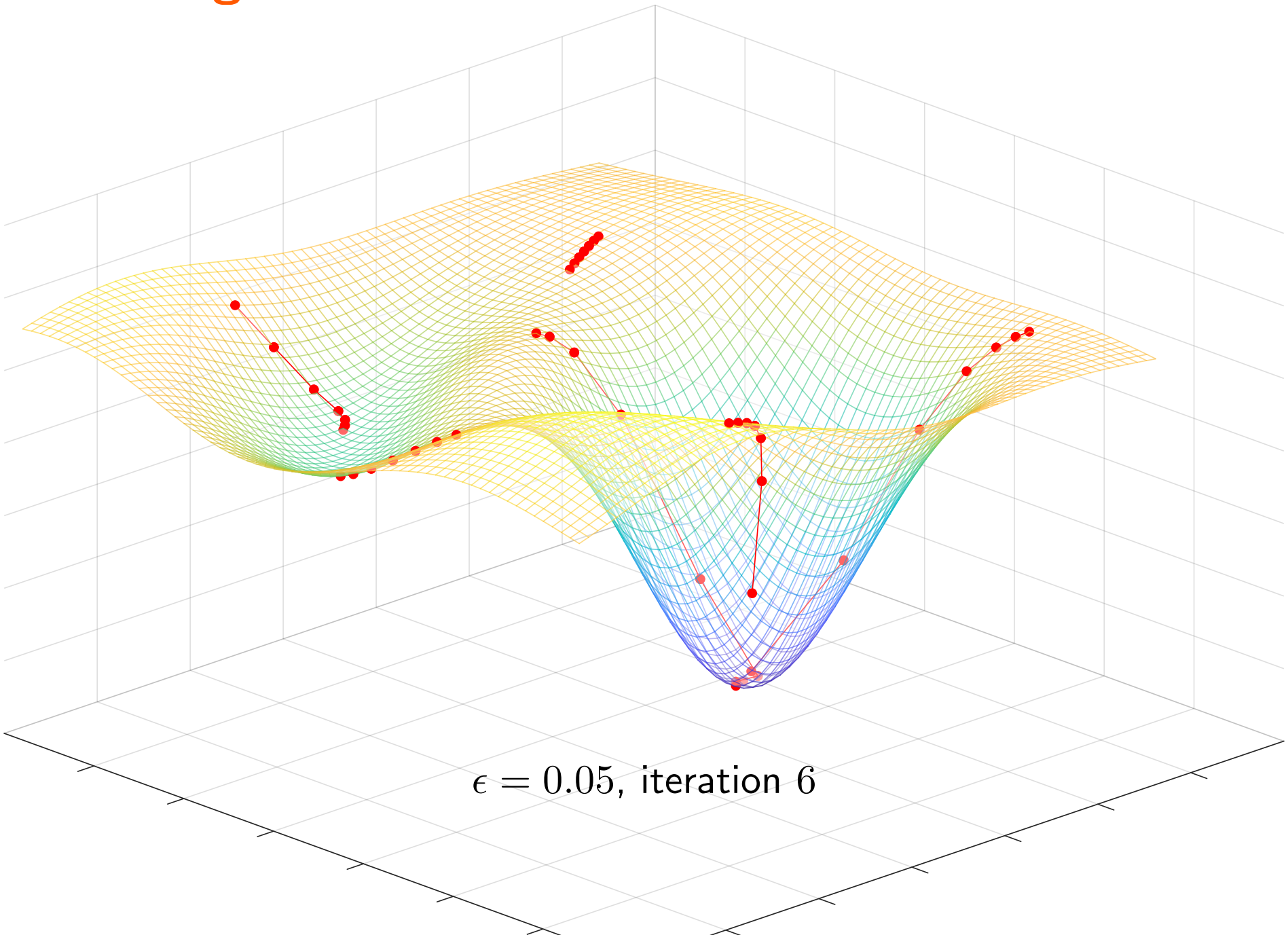


gradient descent in two dimensions



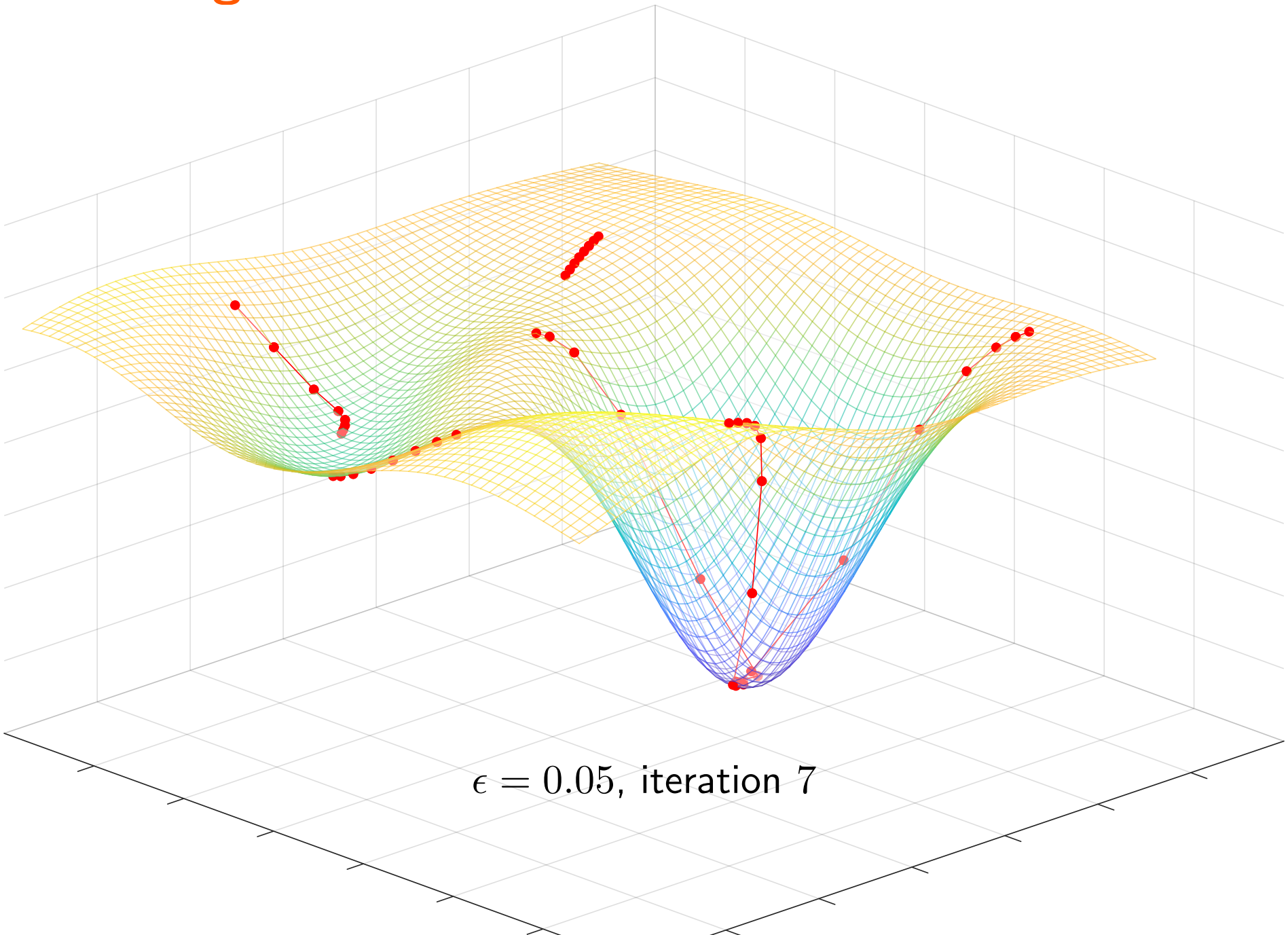
$\epsilon = 0.05$, iteration 5

gradient descent in two dimensions



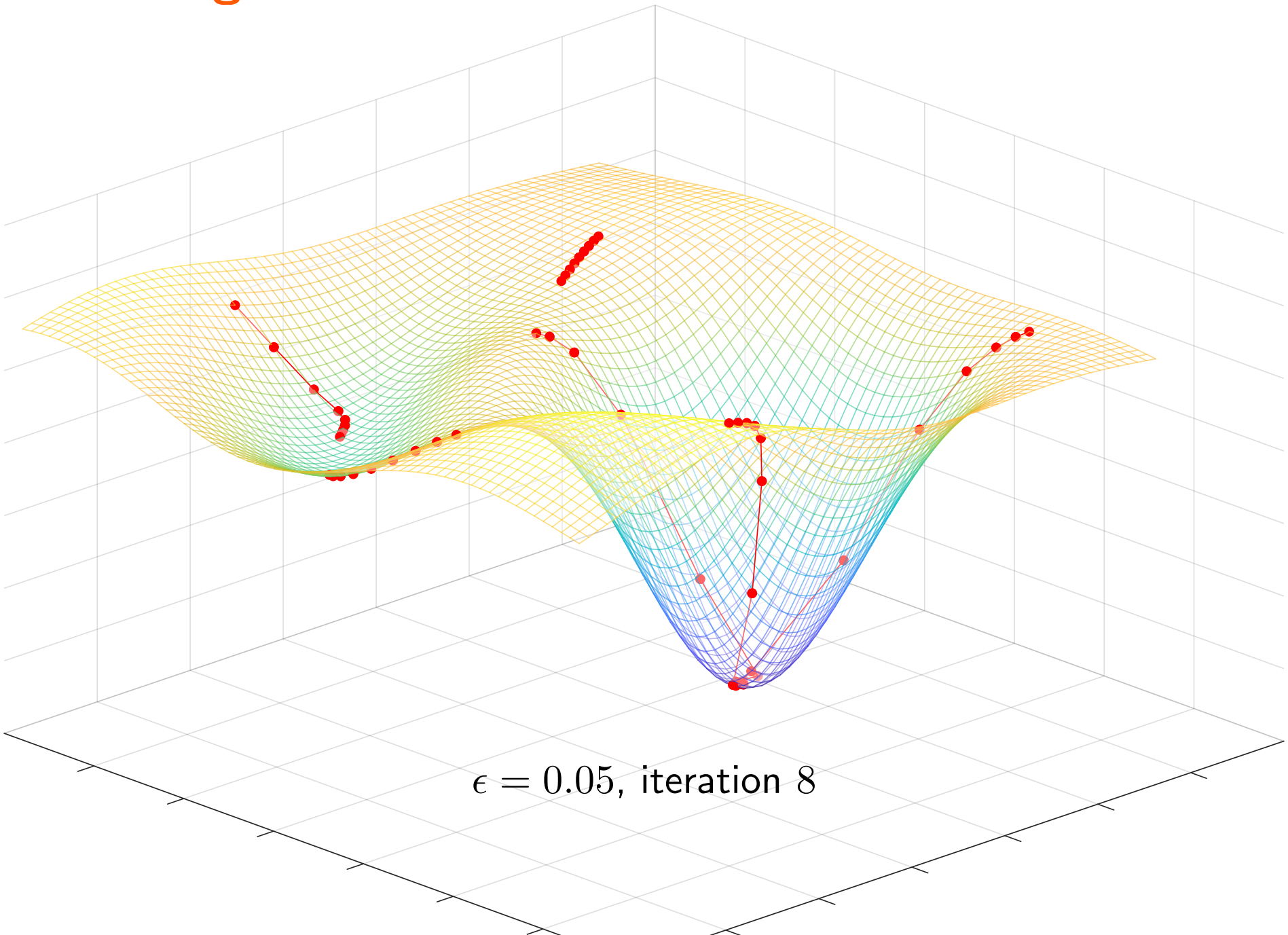
$\epsilon = 0.05$, iteration 6

gradient descent in two dimensions



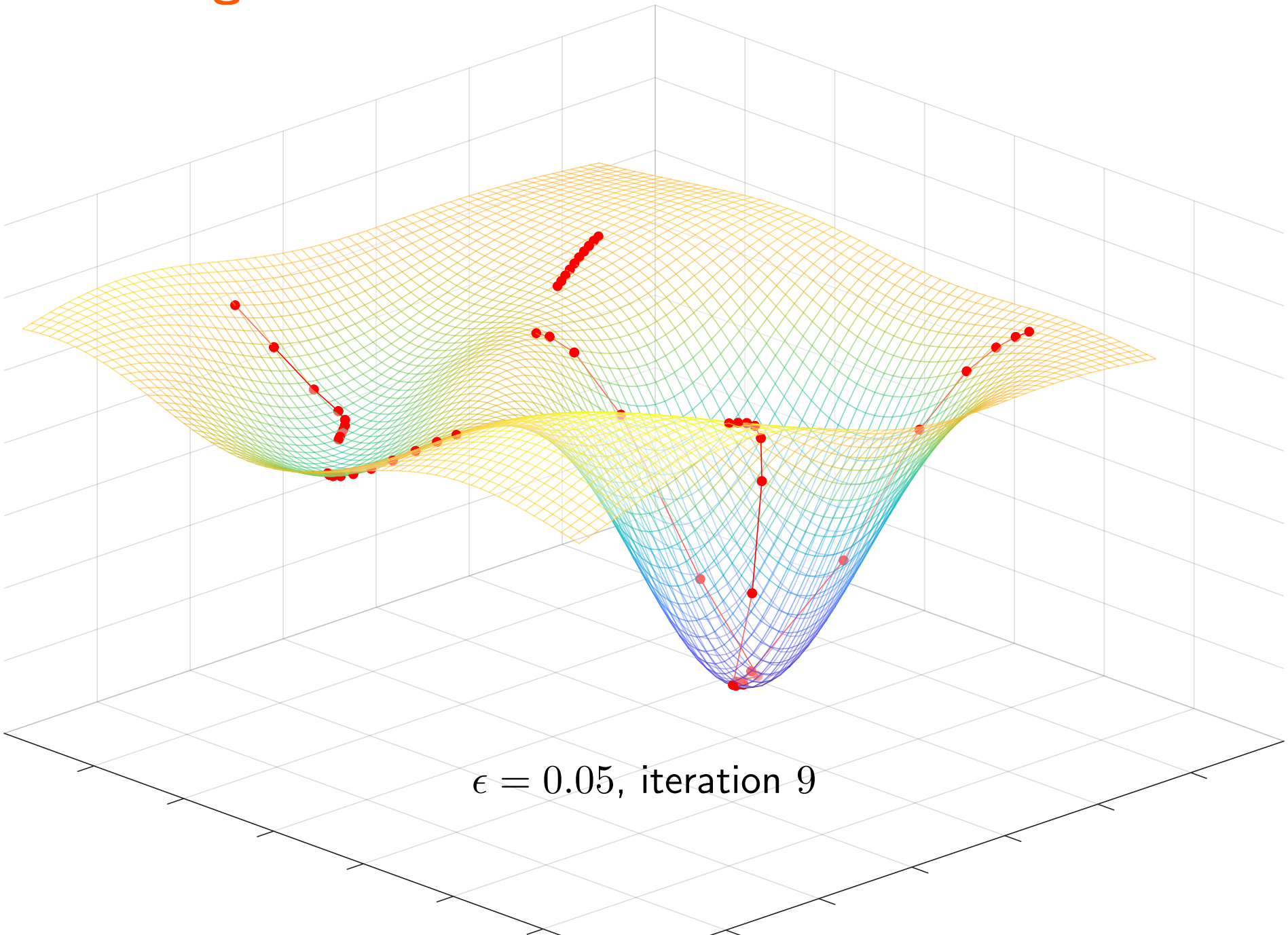
$\epsilon = 0.05$, iteration 7

gradient descent in two dimensions

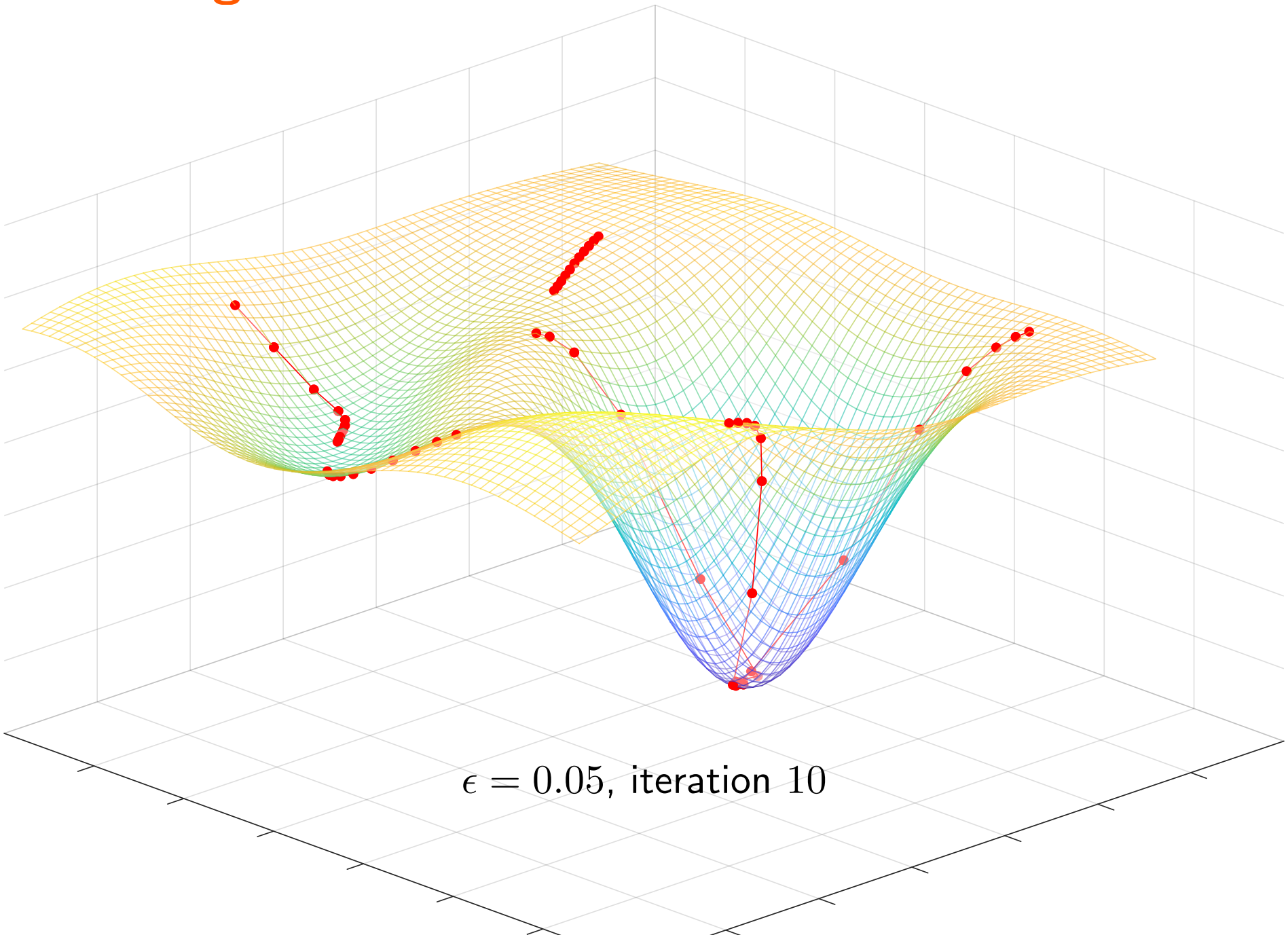


$\epsilon = 0.05$, iteration 8

gradient descent in two dimensions

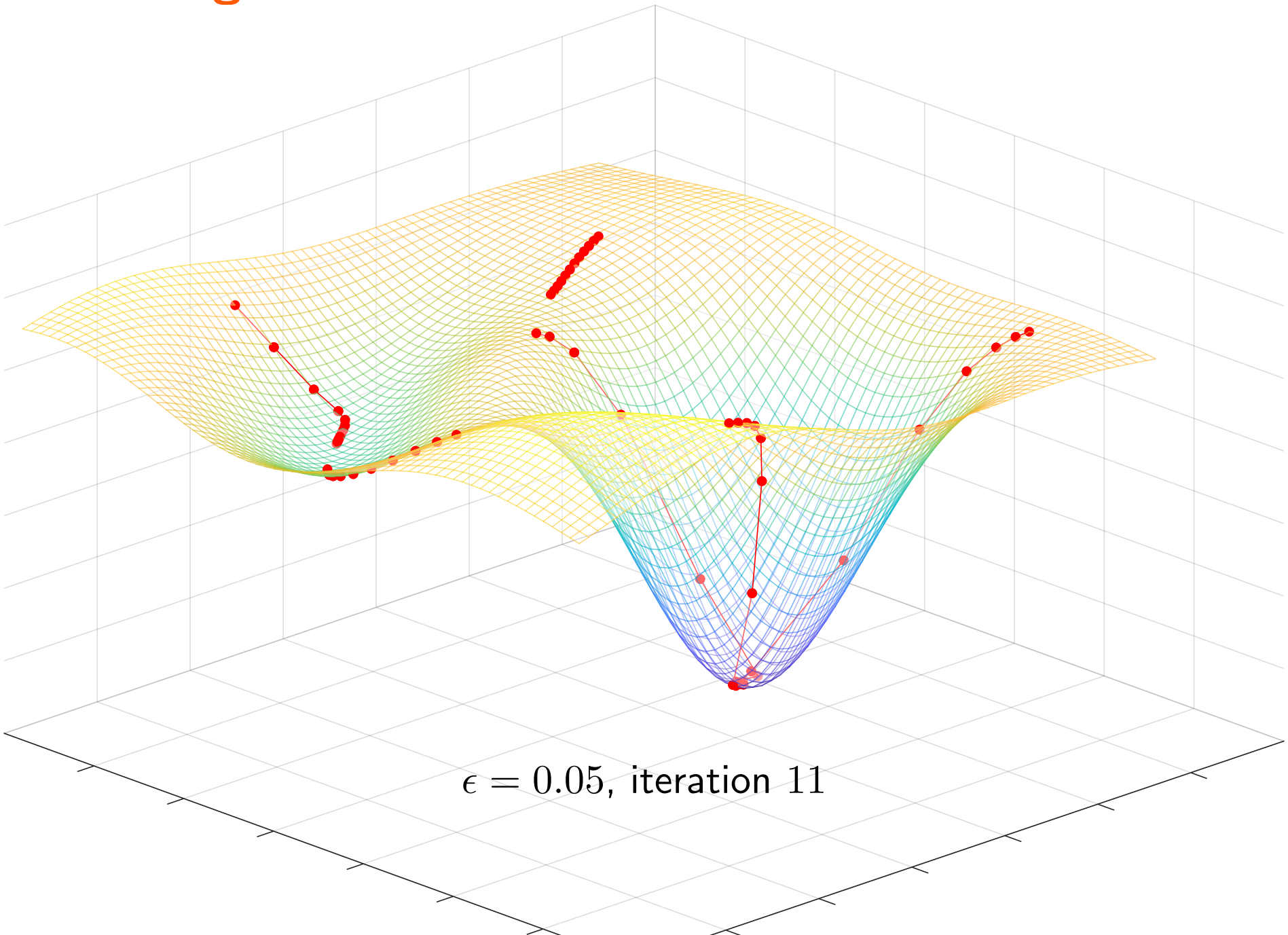


gradient descent in two dimensions



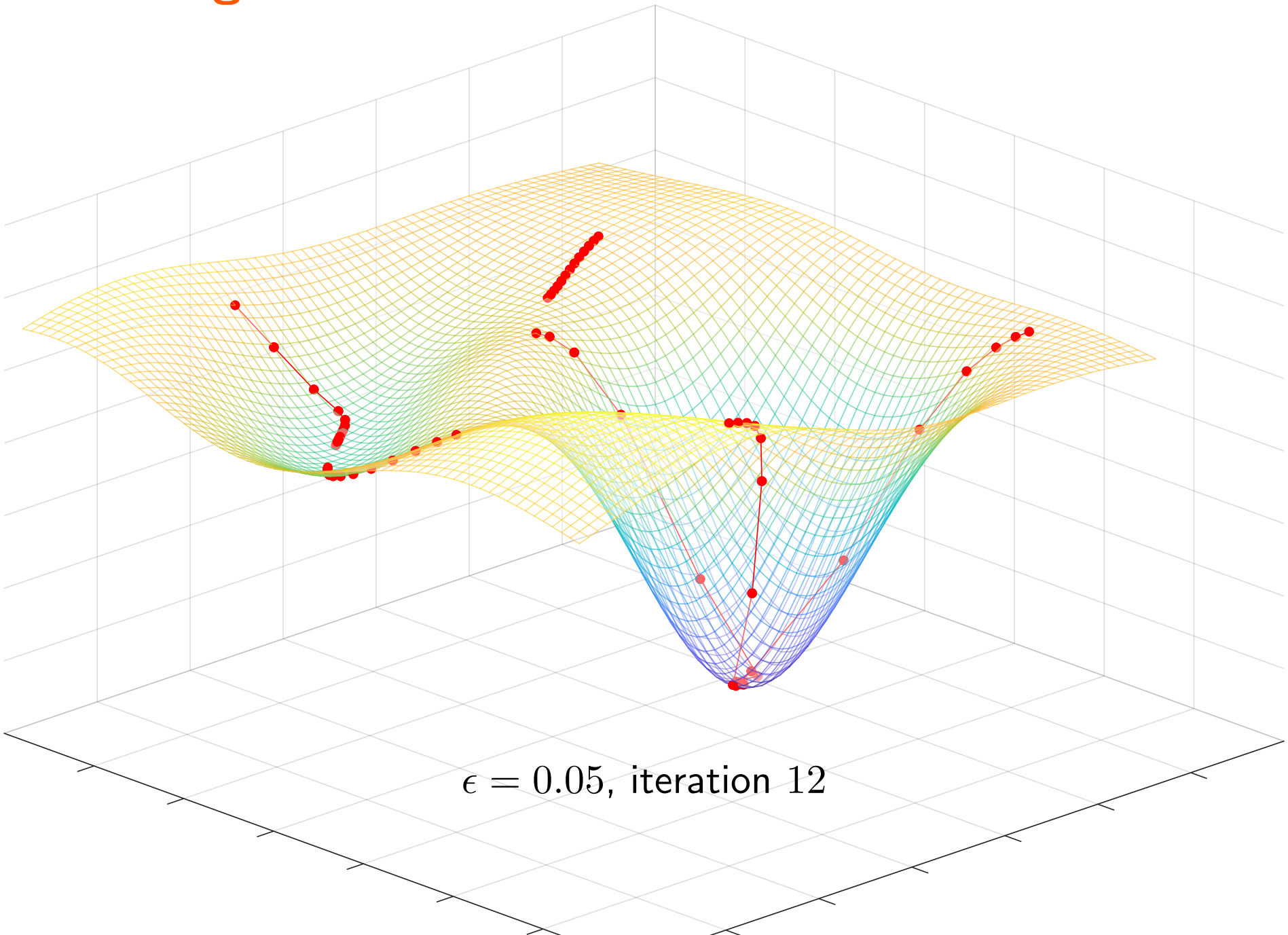
$\epsilon = 0.05$, iteration 10

gradient descent in two dimensions



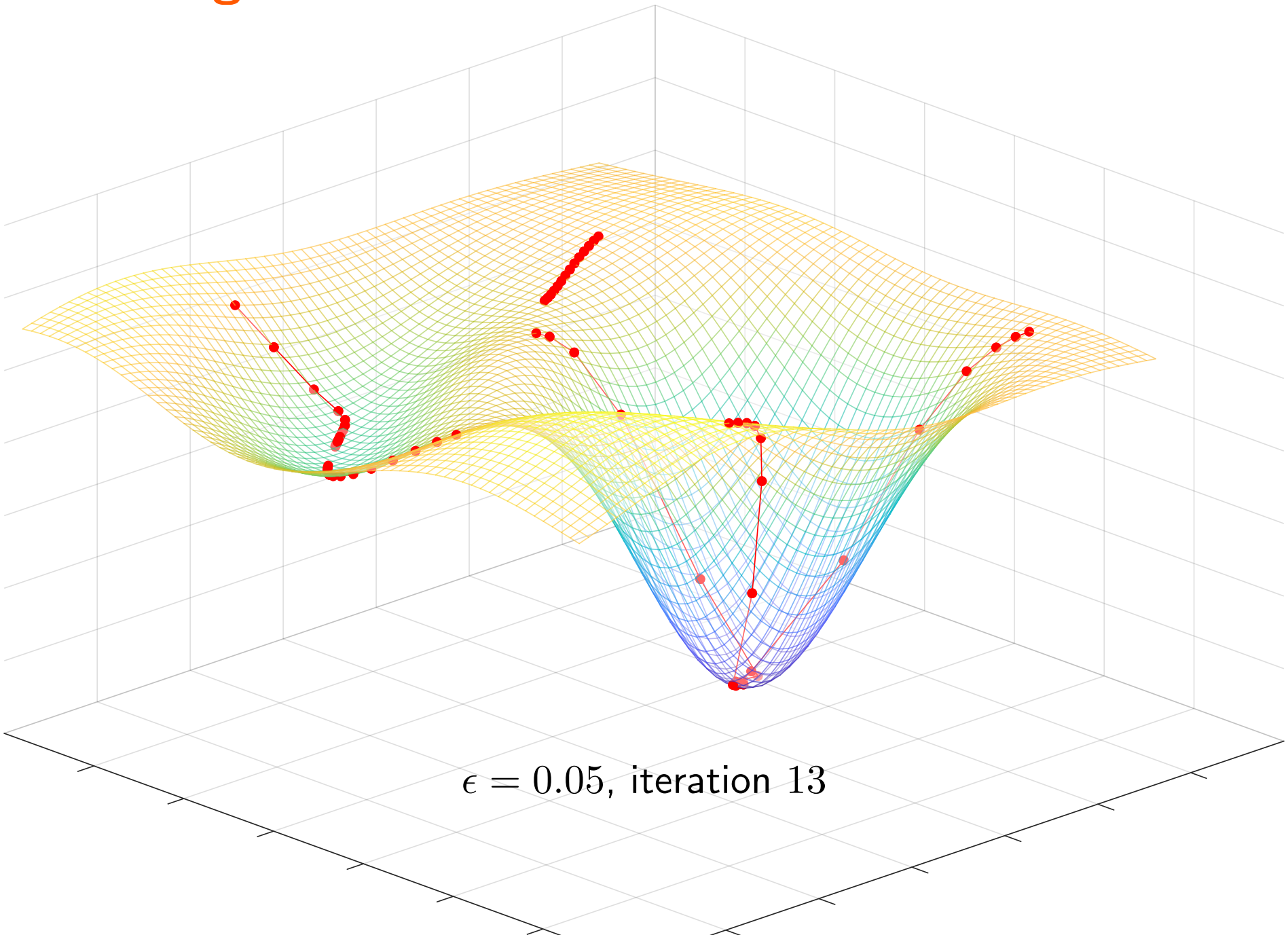
$\epsilon = 0.05$, iteration 11

gradient descent in two dimensions



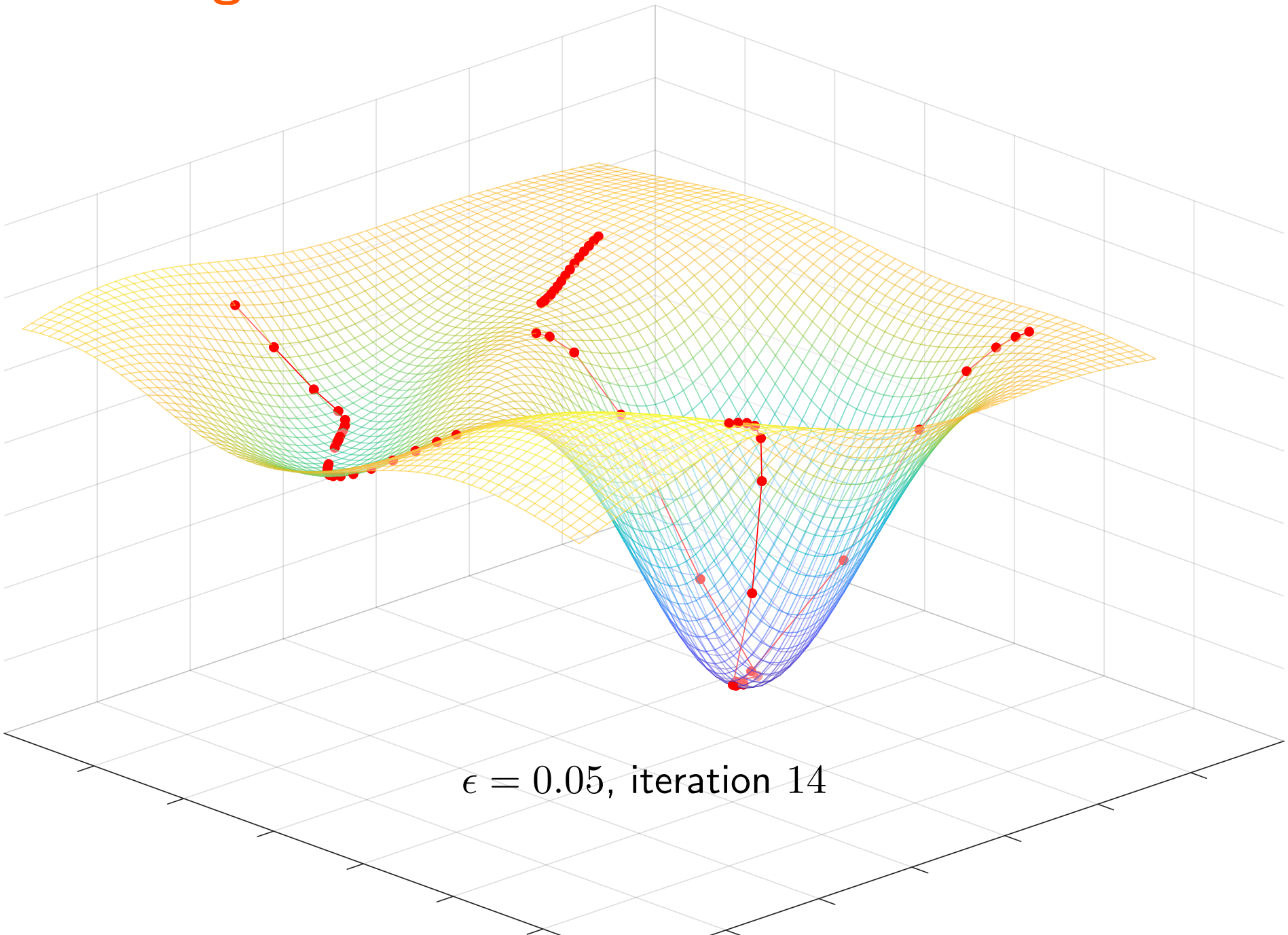
$\epsilon = 0.05$, iteration 12

gradient descent in two dimensions

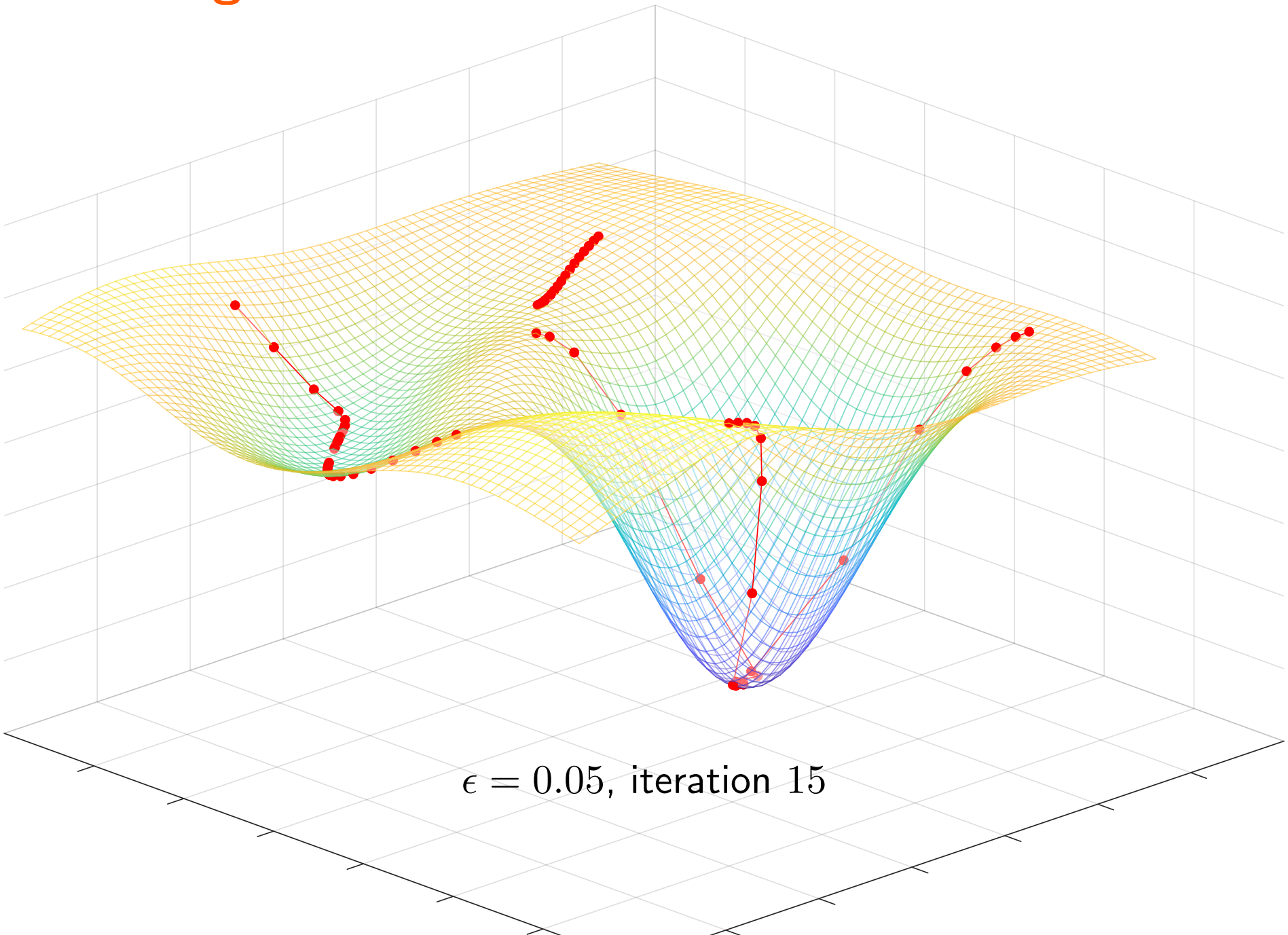


$\epsilon = 0.05$, iteration 13

gradient descent in two dimensions

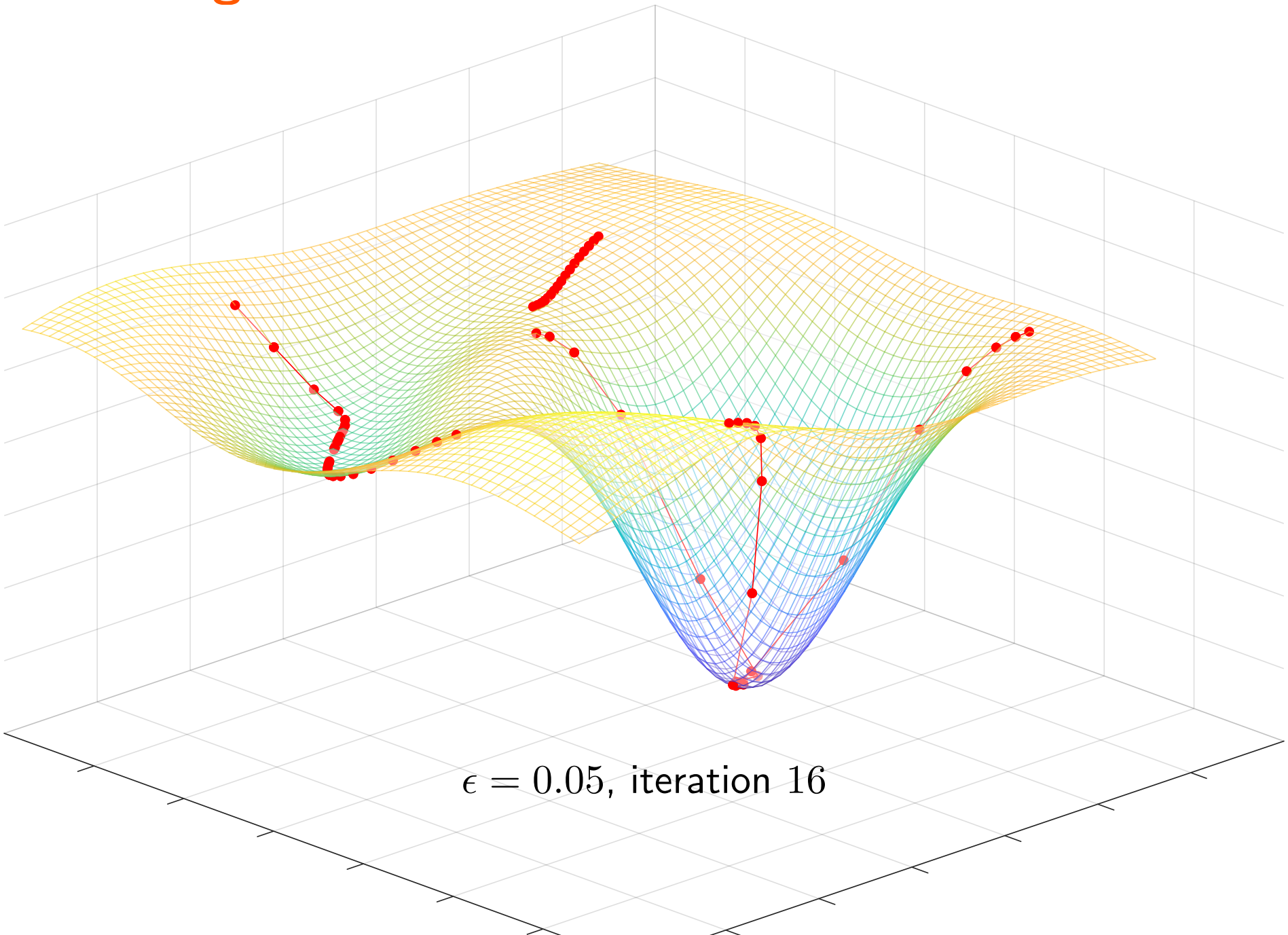


gradient descent in two dimensions



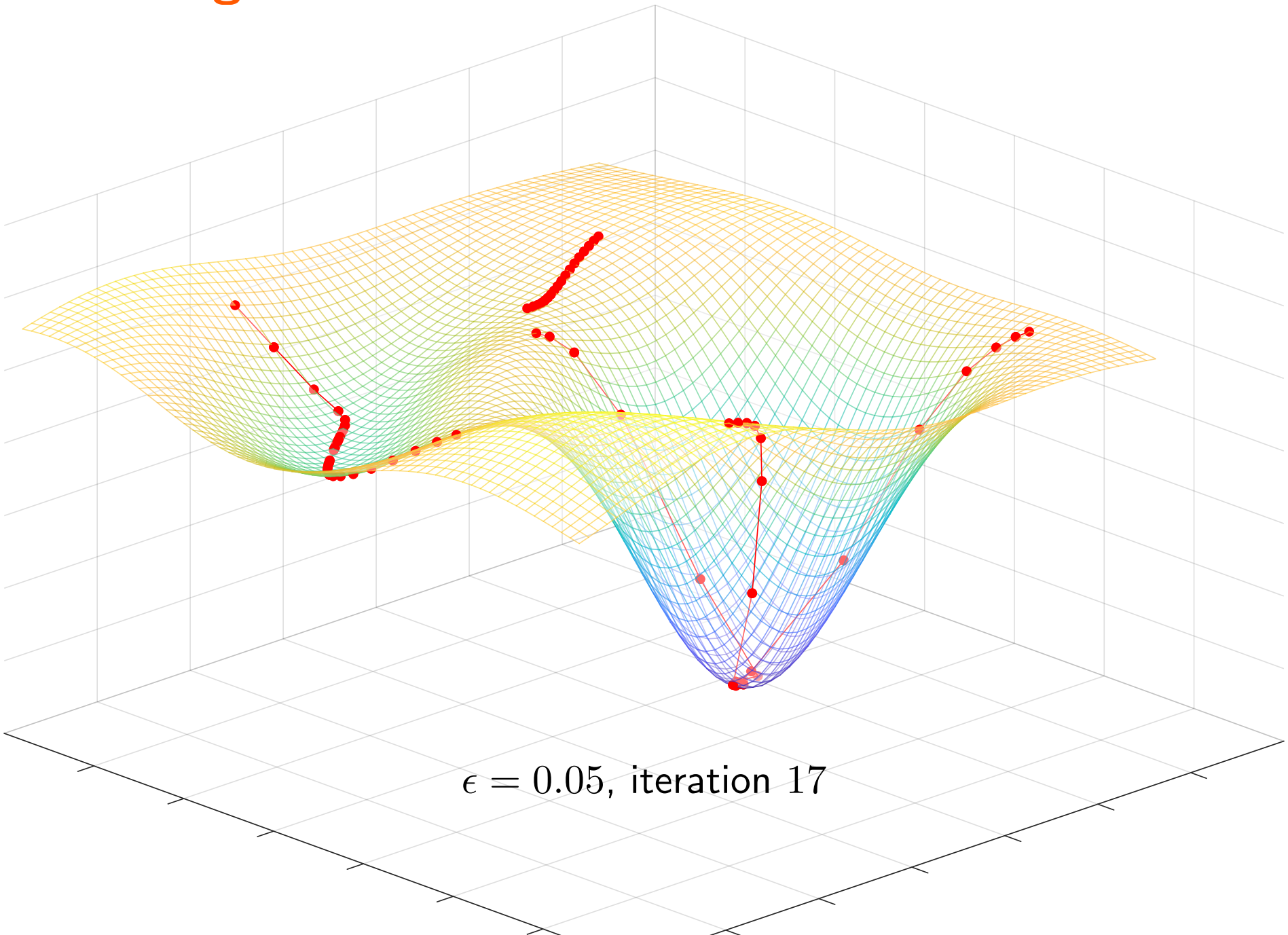
$\epsilon = 0.05$, iteration 15

gradient descent in two dimensions



$\epsilon = 0.05$, iteration 16

gradient descent in two dimensions



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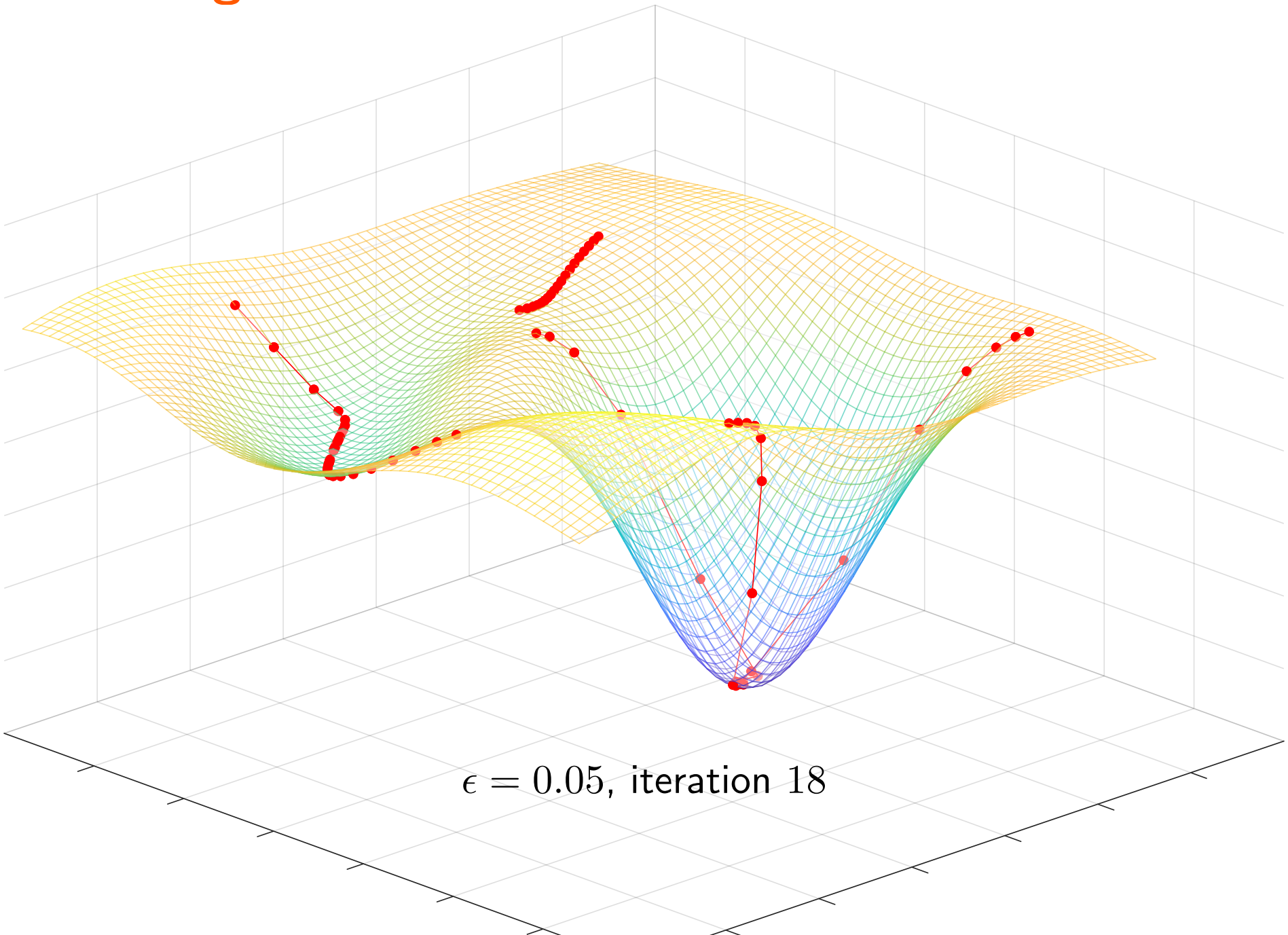
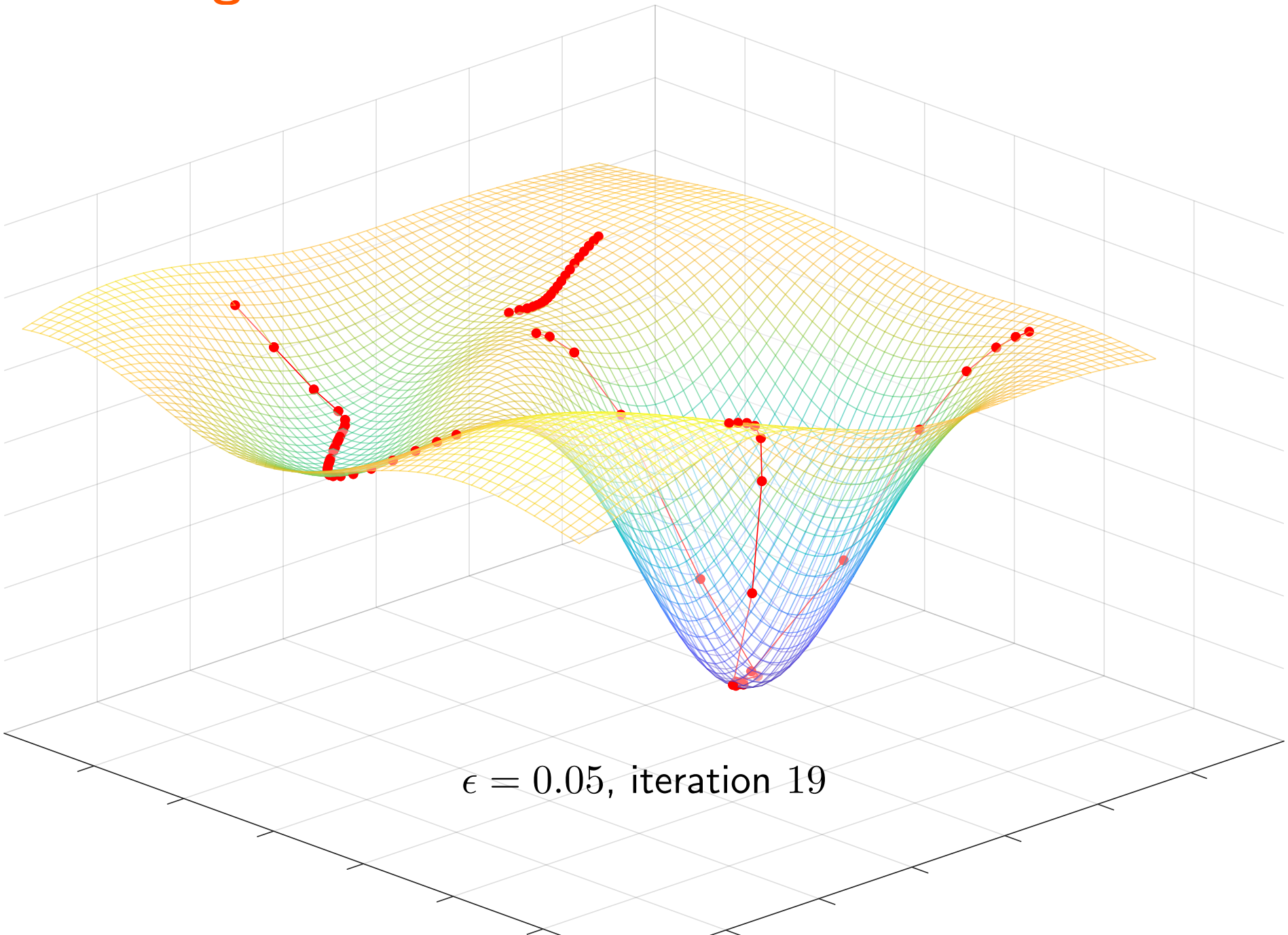
gradient descent in two dimensions



gradient descent in two dimensions



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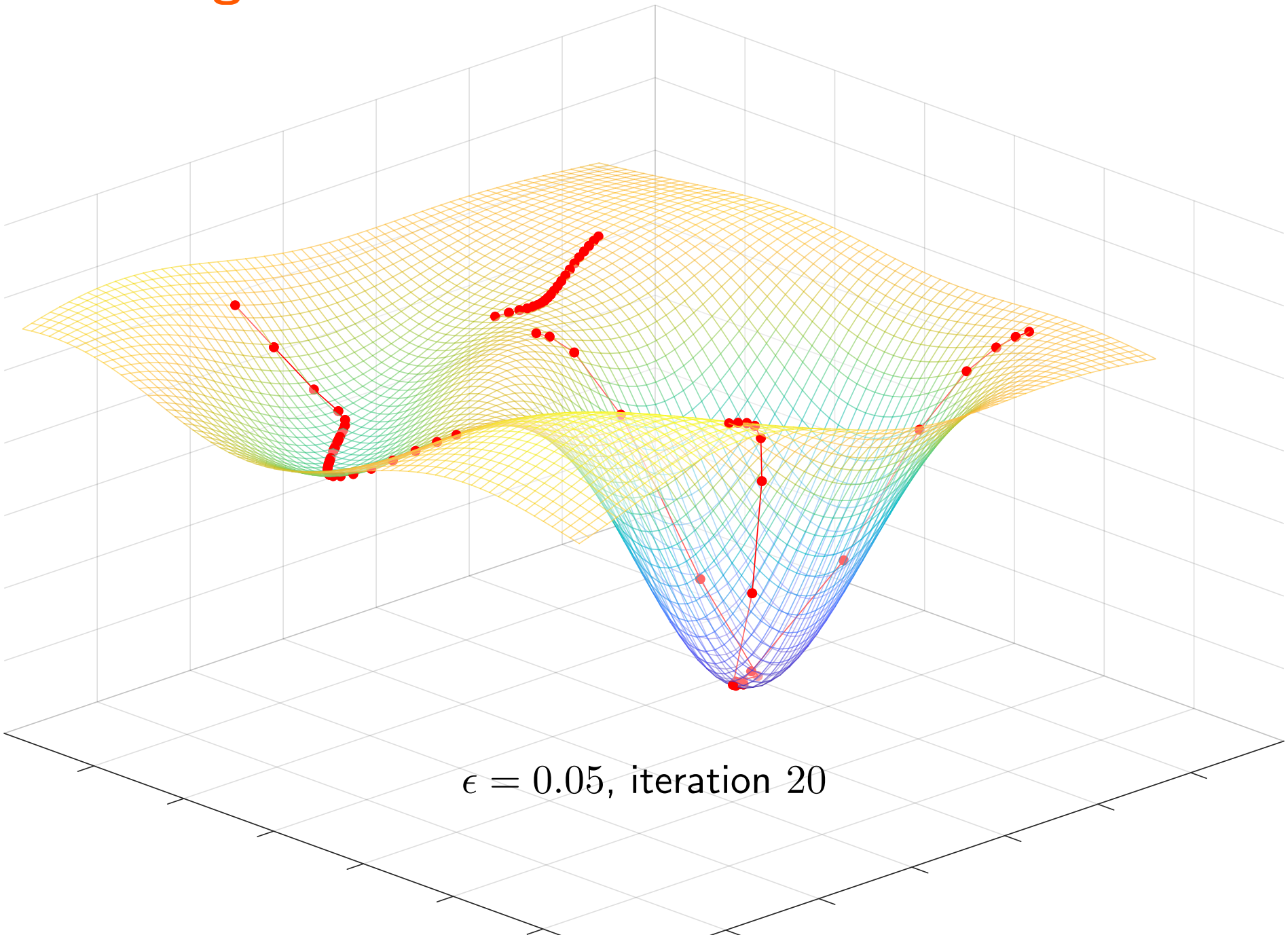

$\epsilon = 0.05$, iteration 20

problems

- f non-convex: local minima
- $d \times d$ Hessian matrix too expensive (d can be millions): unknown curvature
- high condition number: elongated regions
- plateaus, saddle points: no progress
- $\nabla f = \sum_{i=1}^{n} \nabla f_i$ itself too expensive (n can also be millions)

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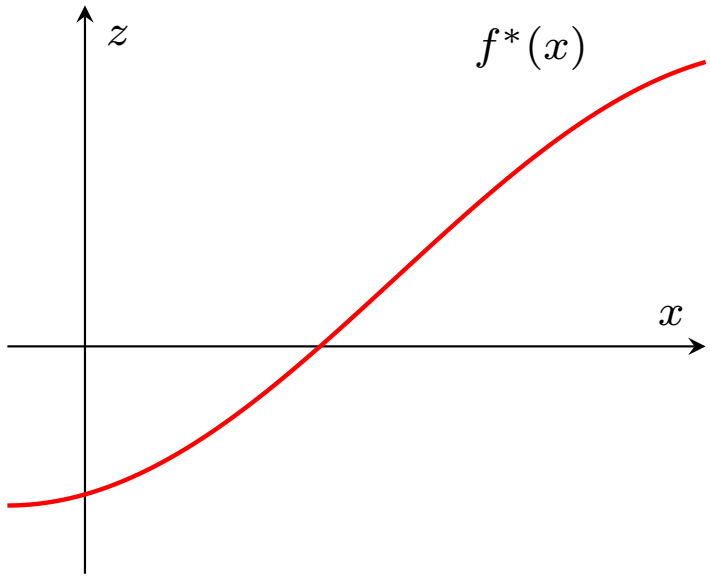
sequential estimation

[Robbins and Monro 1951]



- suppose f^* is the expectation of random variable z conditional on x, and f is its empirical estimate on n samples

$$f^*(x) := \mathbb{E}[z|x] \qquad f(x) := \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$

- we would like to estimate a root x^* of f where $f(x^*) = 0$

Robbins and Monro. AMS 1951. A Stochastic Approximation Method.

sequential estimation

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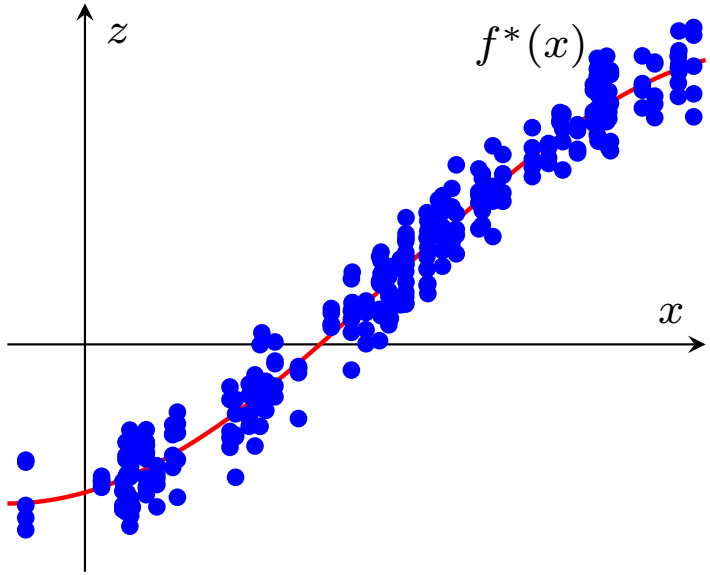

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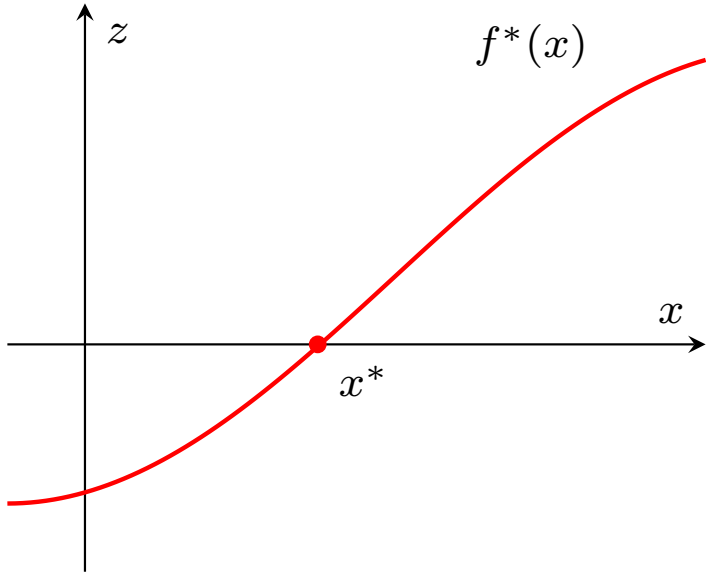

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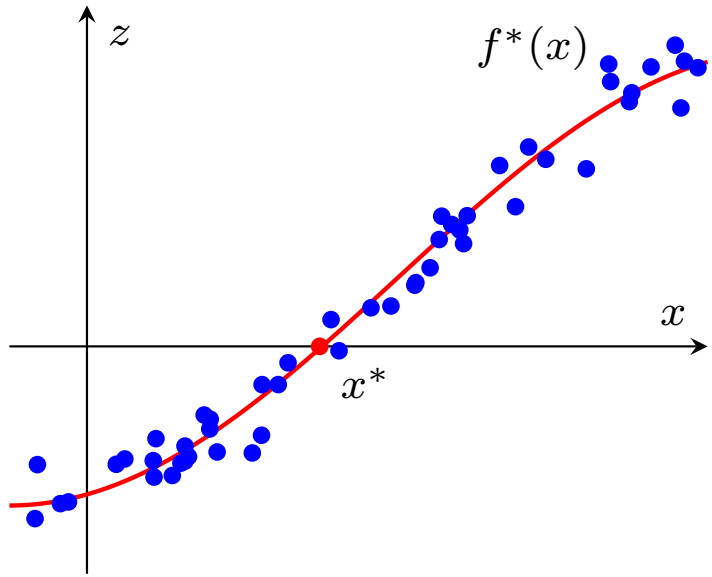

- then we can estimate x^* sequentially

$$x^{(\tau+1)} = x^{(\tau)} - \epsilon_\tau z(x^{(\tau)}) = x^{(\tau)} - \epsilon_\tau f_i(x^{(\tau)})$$

where $z(x^{(\tau)})$ is an observation of z when $x = x^{(\tau)}$ and i is a random index in $\{1, \ldots, n\}$

Robbins and Monro. AMS 1951. A Stochastic Approximation Method.

sufficient conditions for convergence

- successive corrections decrease in magnitude

$$\lim_{\tau \to \infty} \epsilon_\tau = 0$$

- the algorithm does not converge short of the root

$$\sum_{\tau=1}^{\infty} \epsilon_\tau = \infty$$

- the accumulated "noise" has finite variance

$$\sum_{\tau=1}^{\infty} \epsilon_\tau^2 < \infty$$

Robbins and Monro. AMS 1951. A Stochastic Approximation Method.

online gradient descent

- now, replace x by the parameters $\boldsymbol{\theta}$ of our model, and f by ∇E, the gradient of our empirical risk
- the update rule becomes

$$\boldsymbol{\theta}^{(\tau+1)} \leftarrow \boldsymbol{\theta}^{(\tau)} - \epsilon_\tau \nabla E_i(\boldsymbol{\theta}^{(\tau)})$$

- and, under the same conditions, it converges to a root of

$$\nabla E(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \nabla E_i(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \nabla L(f(\mathbf{x}_i; \boldsymbol{\theta}), t_i)$$

  that is, to a local minimum of E
- mini-batch gradient descent is similar but with less "stochastic noise"

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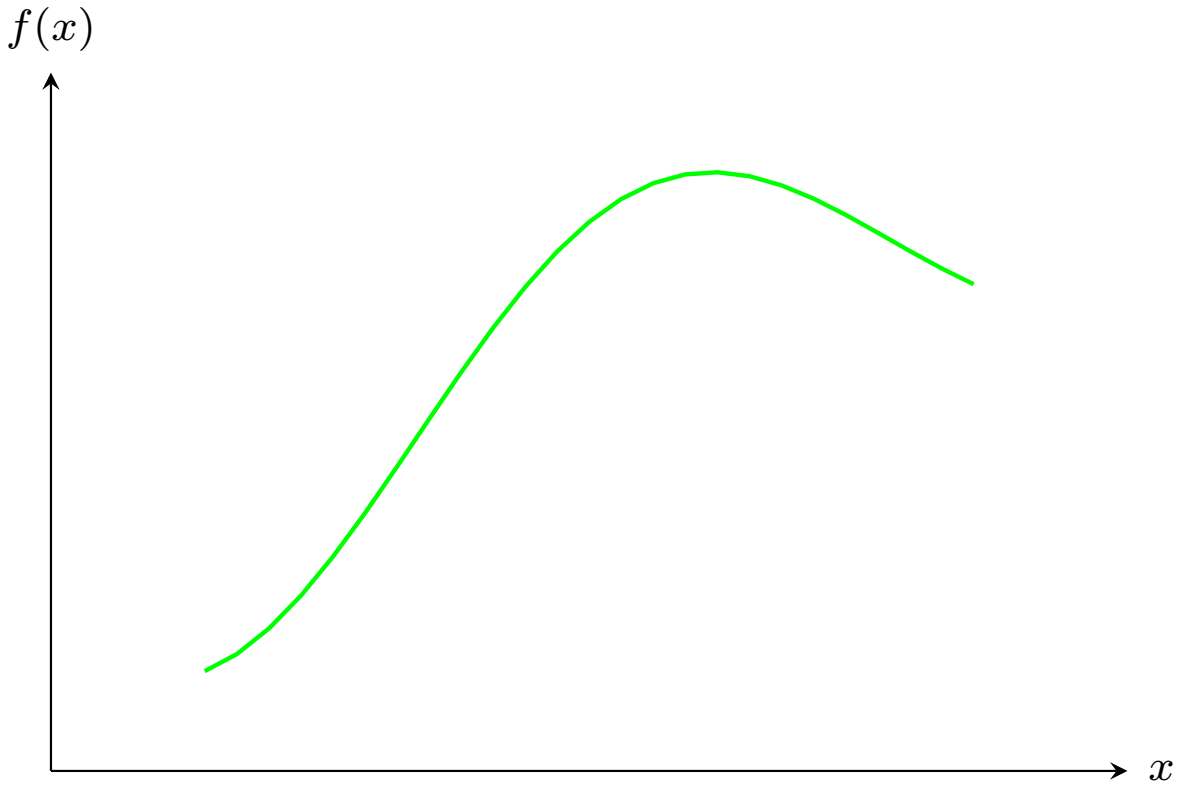
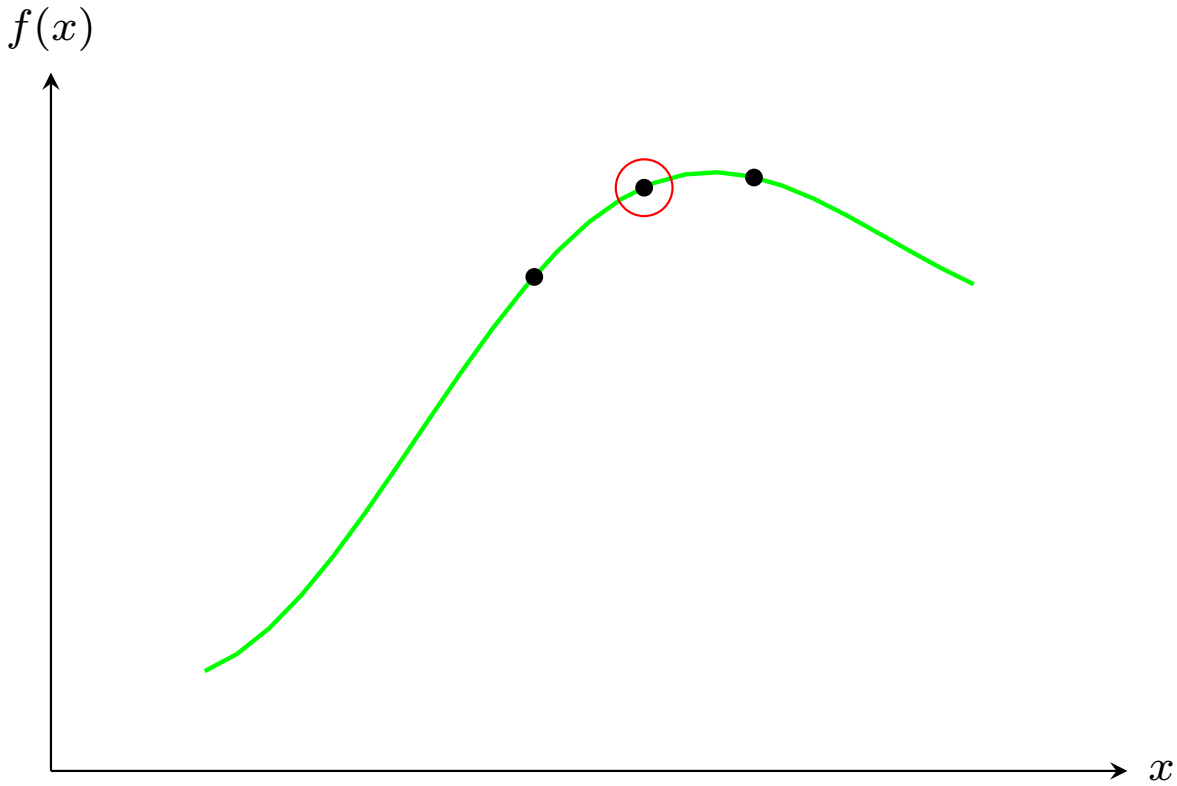
gradient computation

numerical approximation



numerical approximation



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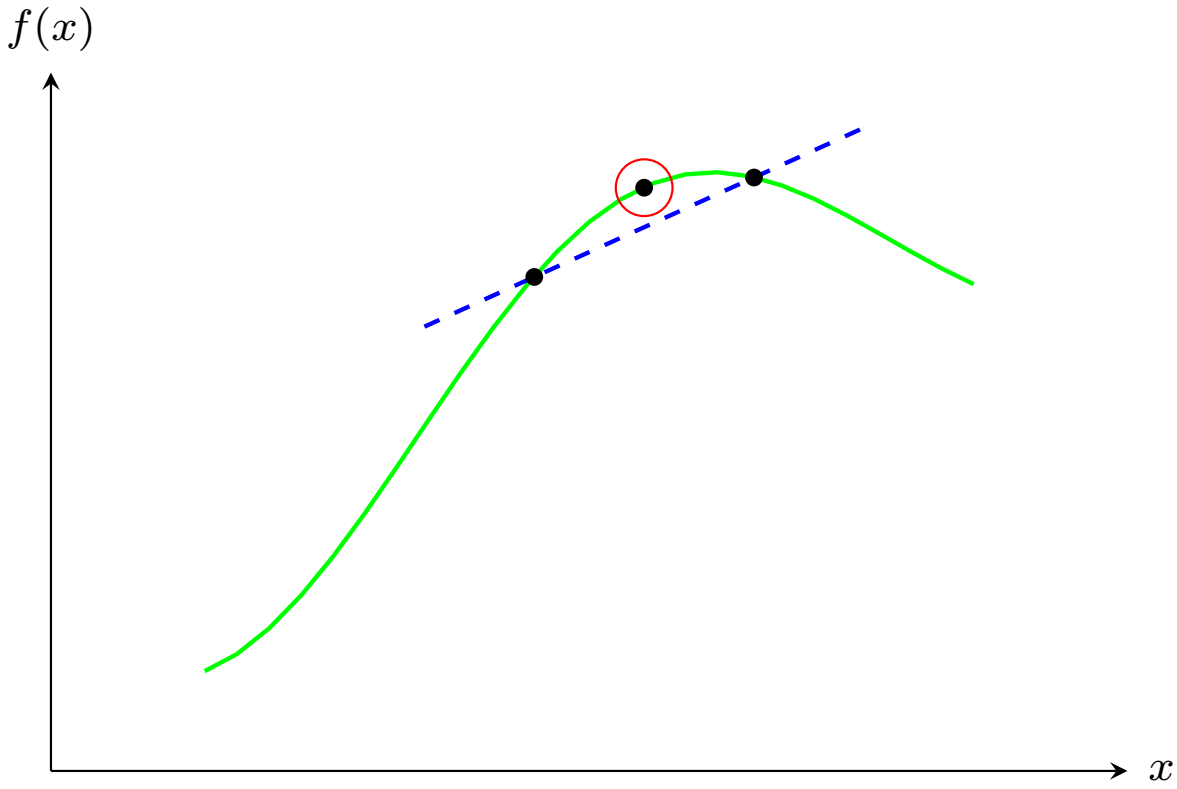

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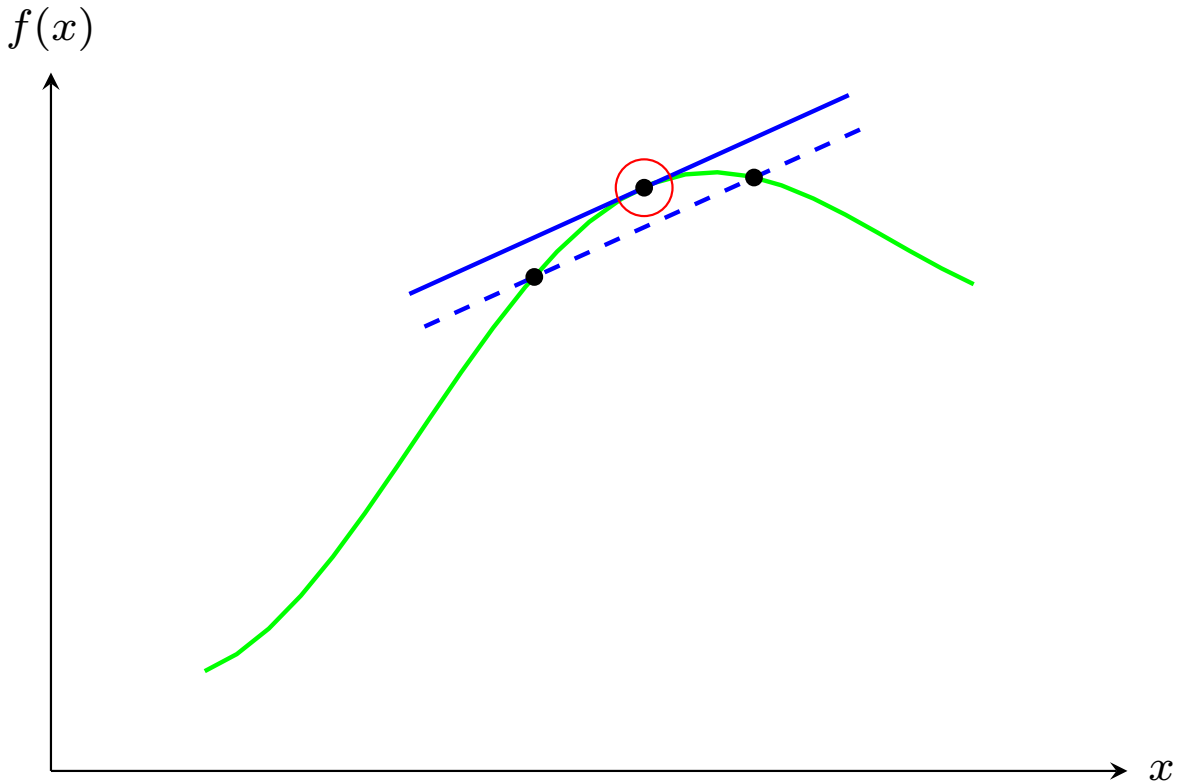

$$\frac{df}{dx}(x) \approx \frac{f(x+\delta) - f(x-\delta)}{2\delta}$$

numerical approximation

- given $f : \mathbb{R}^p \to \mathbb{R}$, its gradient is the vector function

$$\nabla f := \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_p} \right)$$

we also write

$$\nabla f = Df := (D_1 f, \ldots, D_p f)$$

- and each partial derivative $D_i f$ can be approximated at $\mathbf{x}$ by symmetric difference formula

$$\Delta_i f(\mathbf{x}; \delta) := \frac{f(\mathbf{x} + \delta \mathbf{e}_i) - f(\mathbf{x} - \delta \mathbf{e}_i)}{2\delta}$$

for small $\delta > 0$, where $\mathbf{e}_i$ the i standard basis vector of $\mathbb{R}^m$

- in practice, the smallest δ should be used that does not cause numerical issues, *e.g.* $\delta \in [10^{-10}, 10^{-5}]$ for double-precision arithmetic

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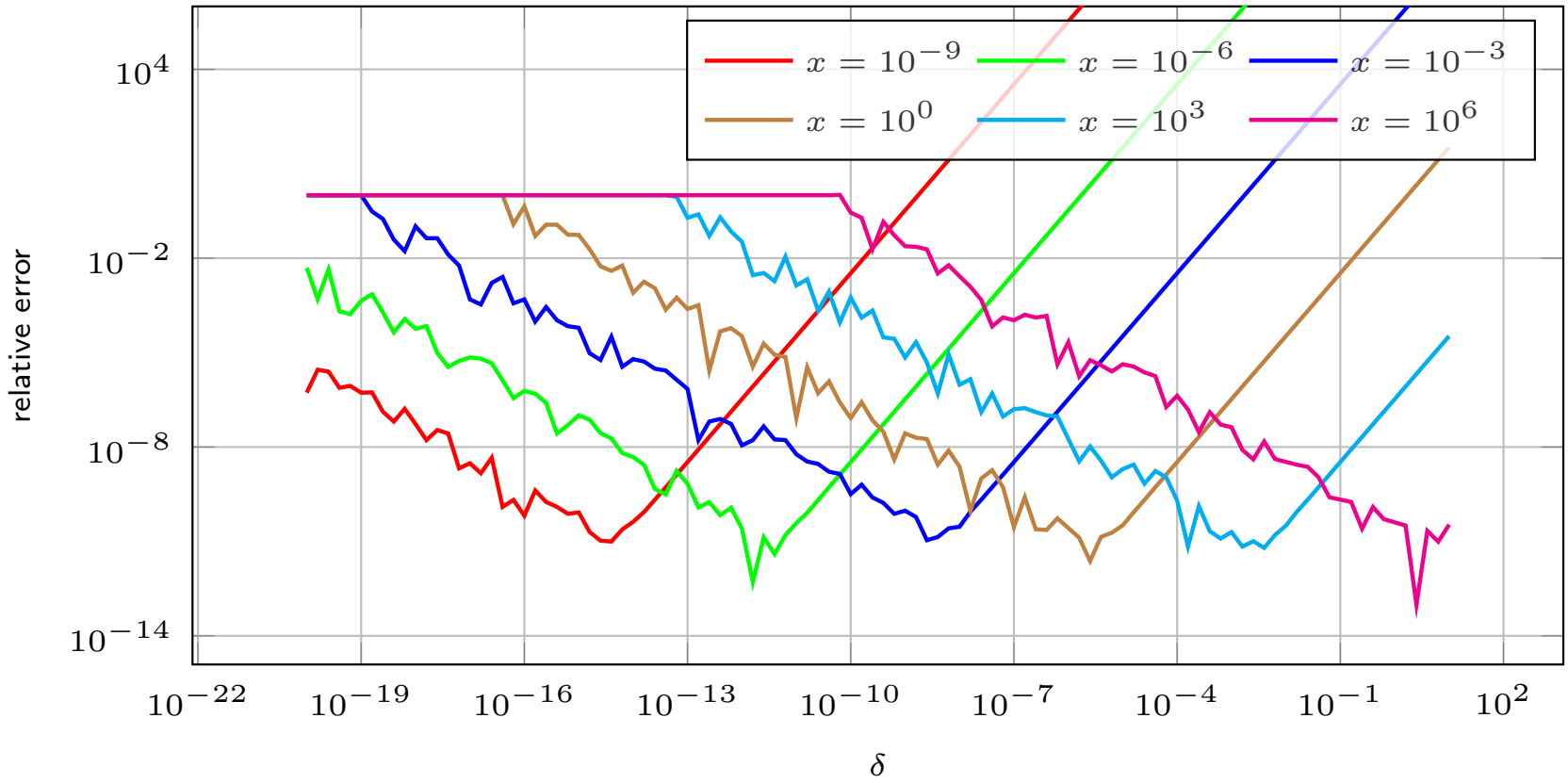
example



- relative error for $f(x) = x^3$, $Df(x) = 3x^2$

$$\frac{|\Delta f(x;\delta) - Df(x)|}{Df(x)}$$

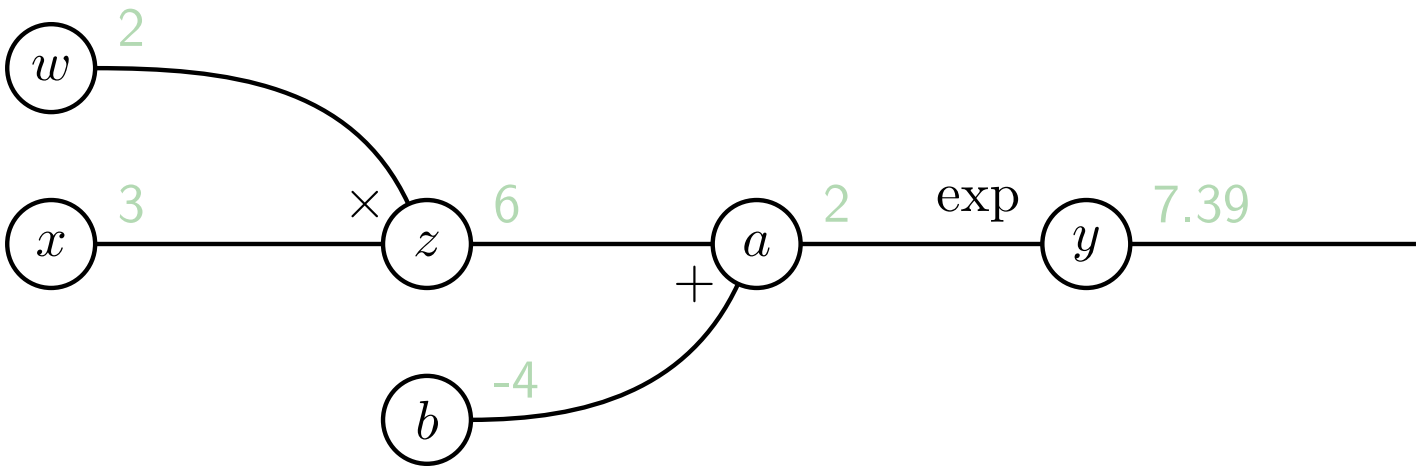
numerical vs. analytical

- apart from accuracy issues, the numerical approximation is impractical in high dimensions: one evaluation of Δf requires $2p$ evaluations of f, and dimension p is easily in the order of millions
- we turn to analytical computation of the gradient, which costs roughly as much as one evaluation of f
- but the numerical approximation always remains useful for double-checking

analytical computation

- all derivatives we care about are the derivatives of the error function with respect to the model parameters: the error function is scalar and we need its gradient
- we are going to write the error function as a composition of simpler functions, and use the chain rule to compute the gradient efficiently
- the error function can be as complex as a program with control flow statements
- each component function, called a unit, is assumed to be at least piecewise differentiable with a known formula for its derivative
- a unit may be a vector function, so we need Jacobian matrices in general, not just gradients

example



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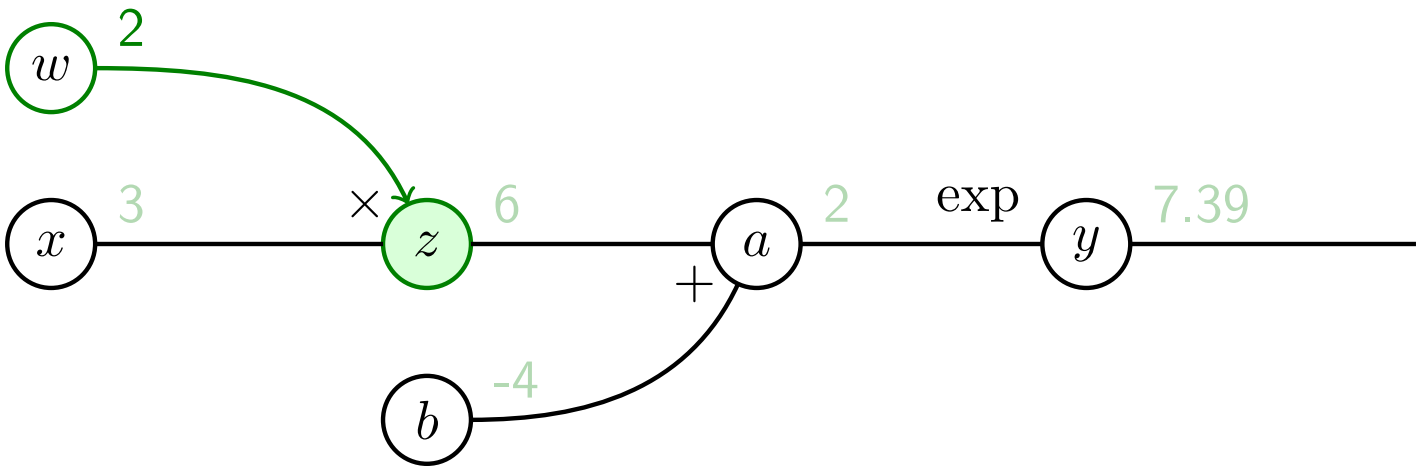

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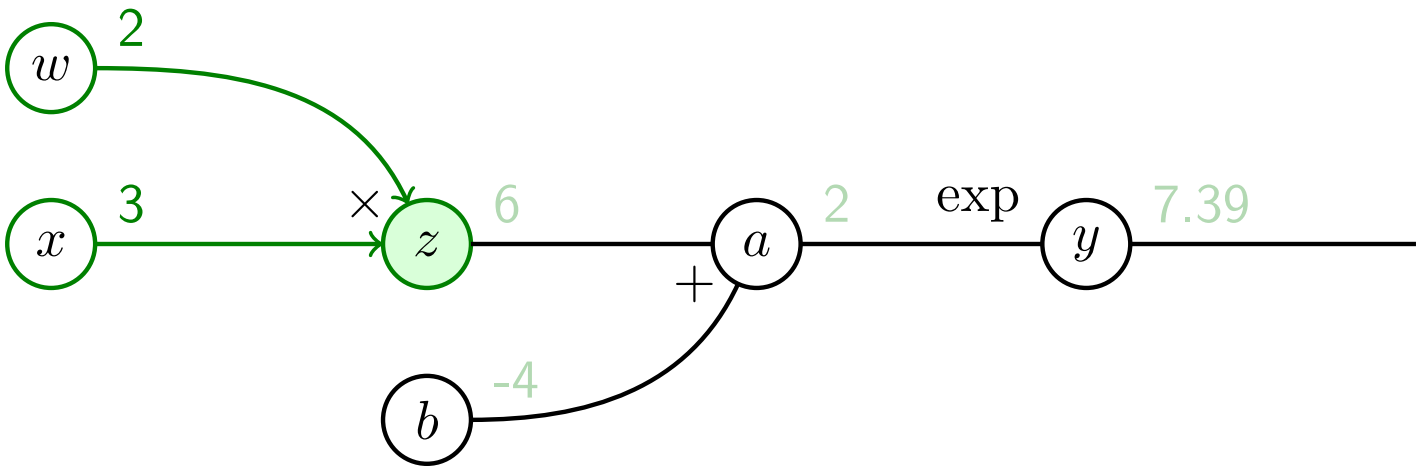

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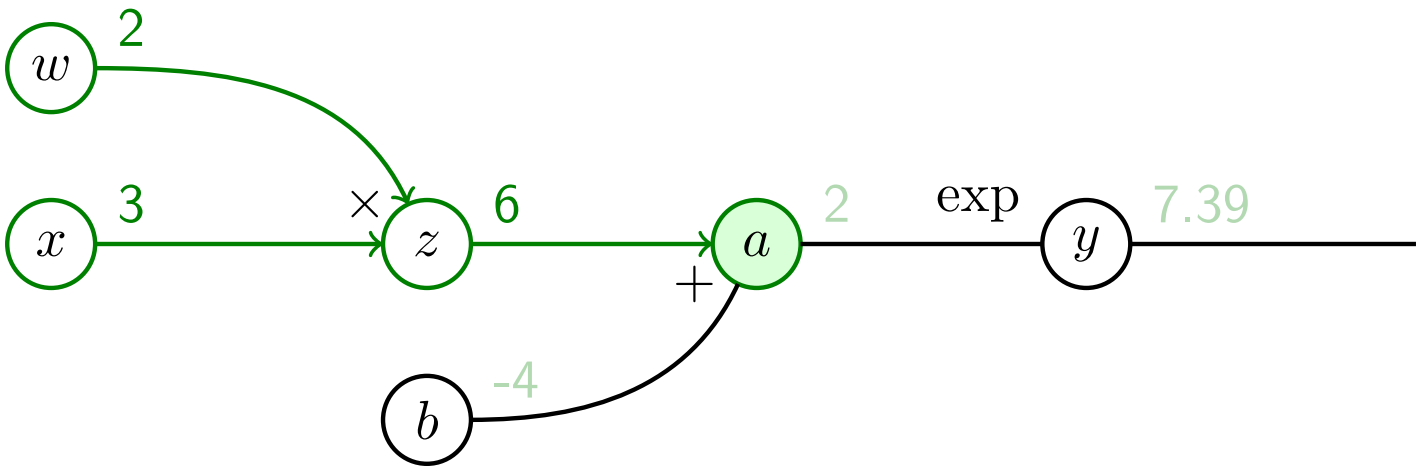

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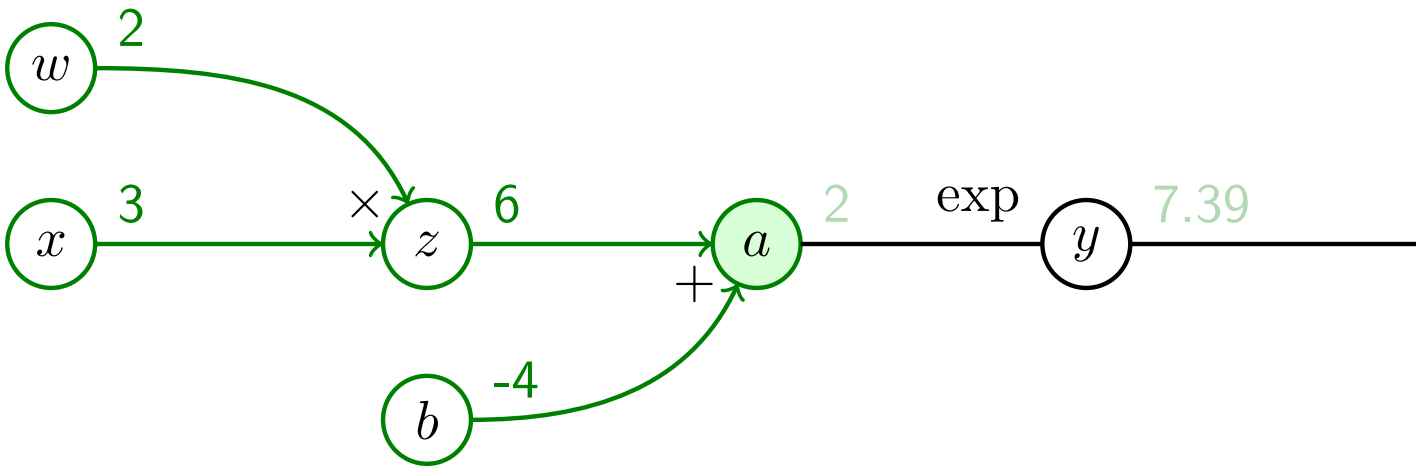

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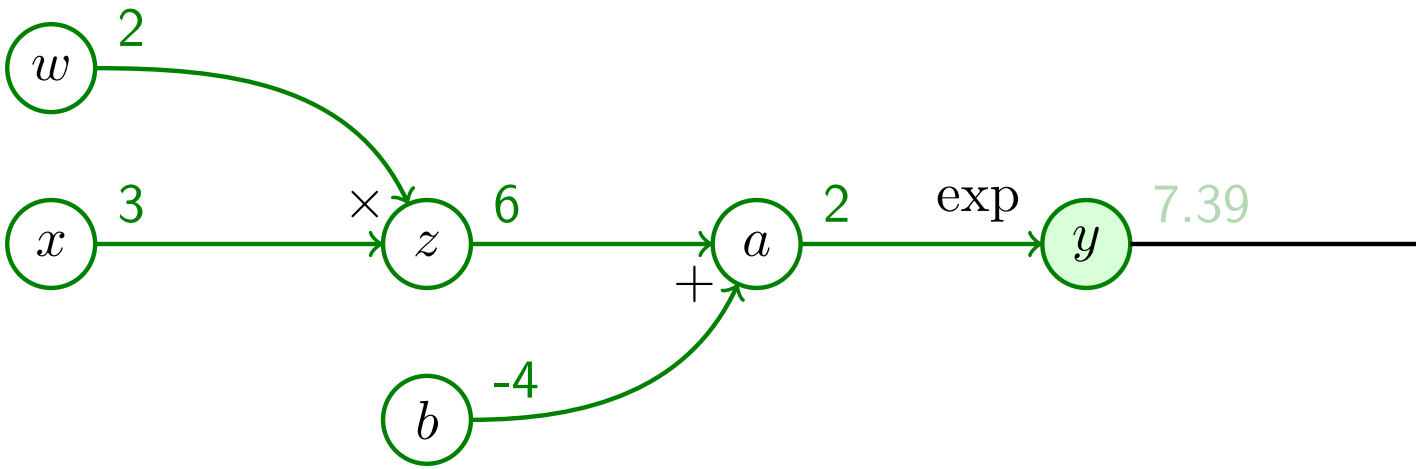

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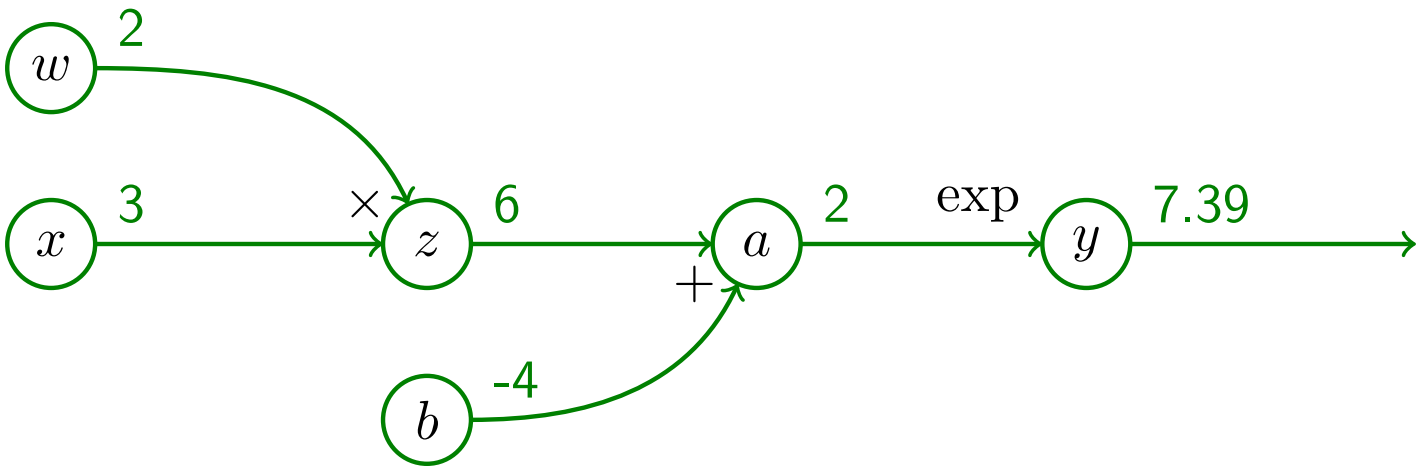

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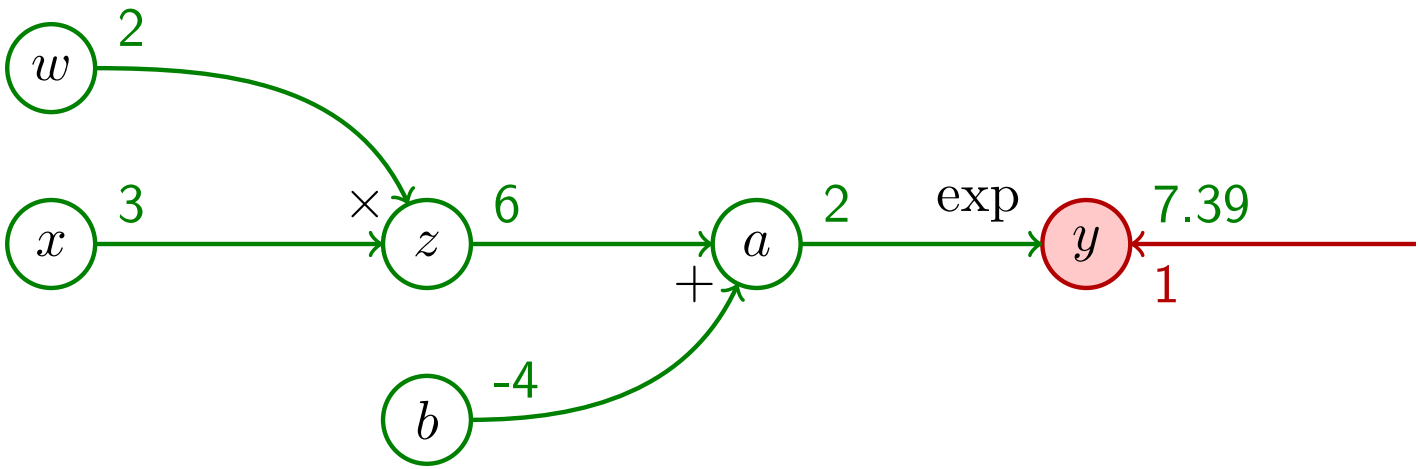

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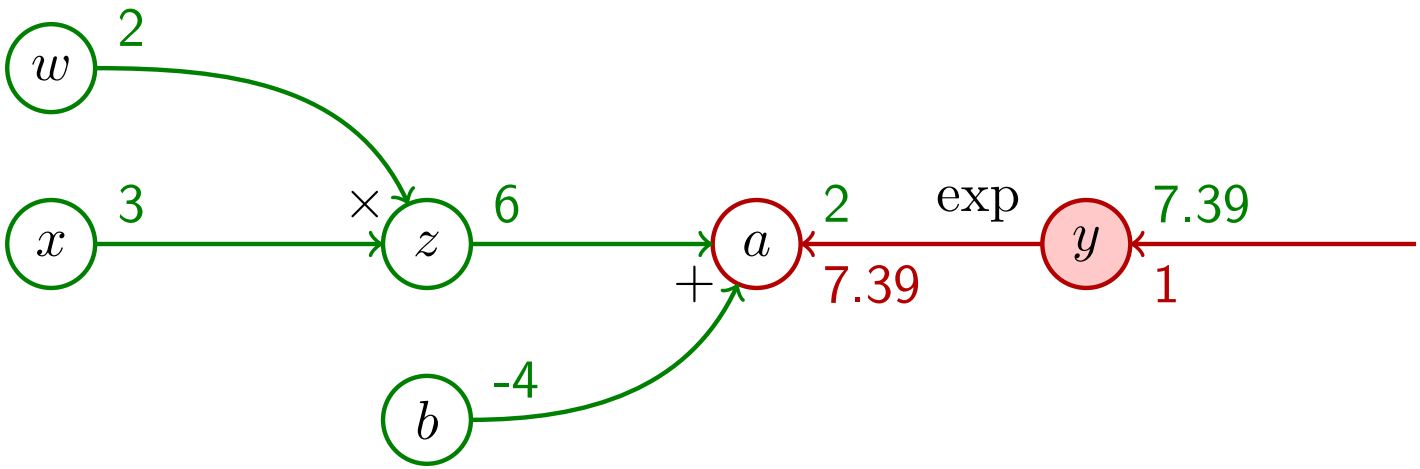

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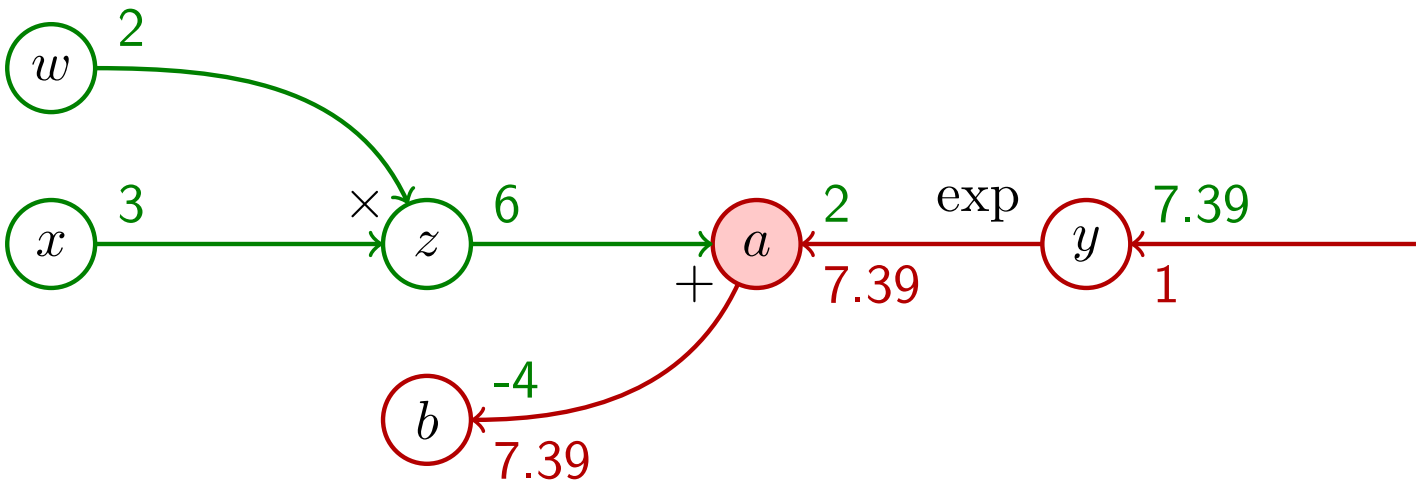

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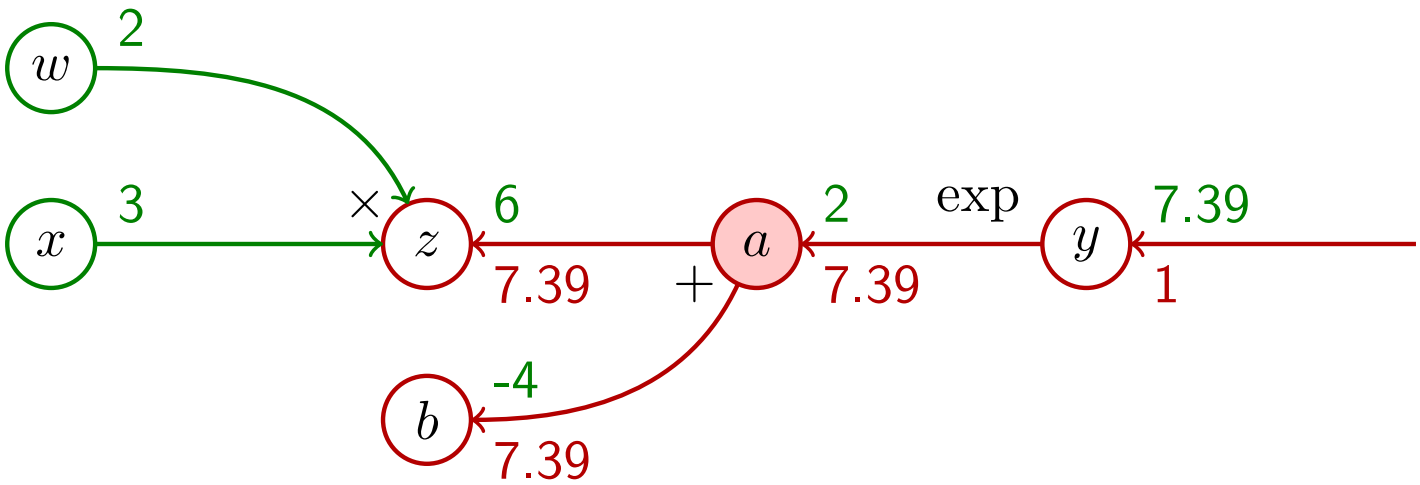

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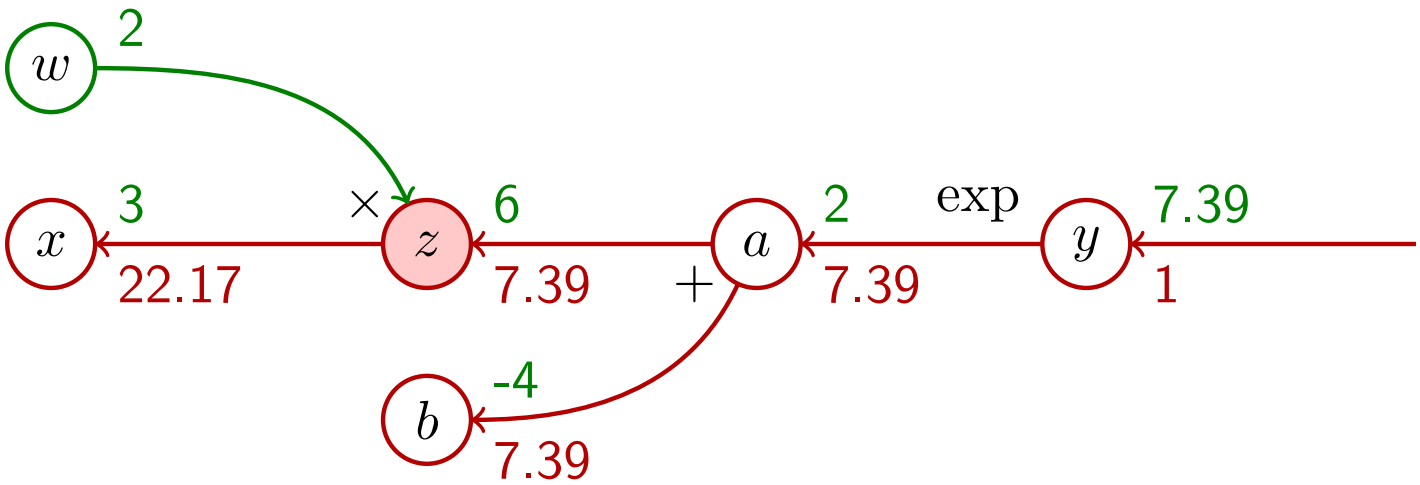

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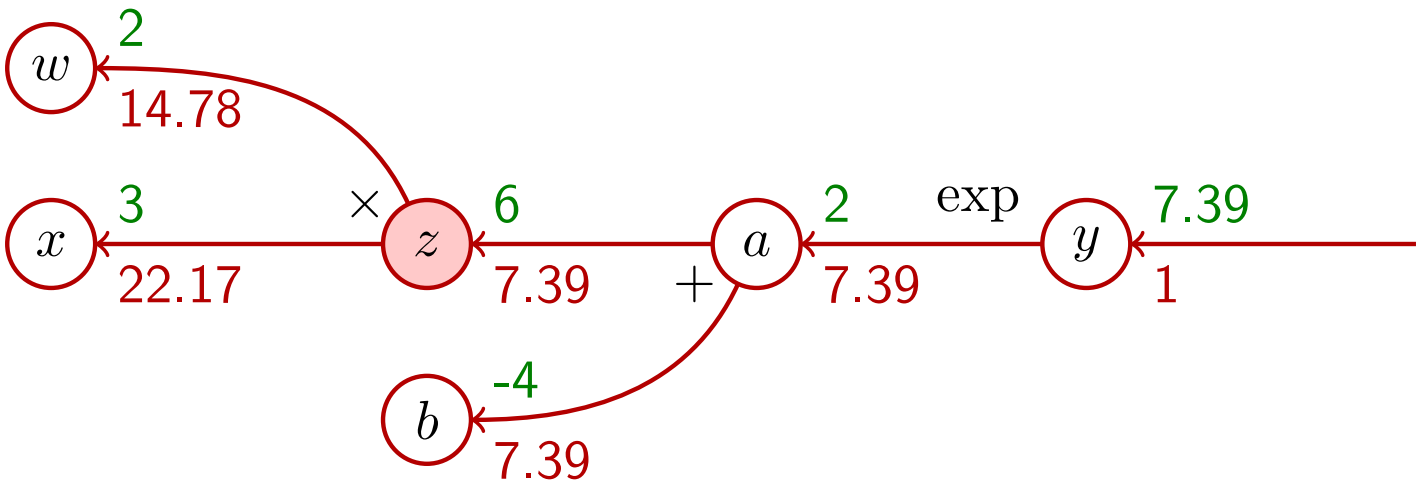

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vector functions

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$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial f}{\partial \mathbf{x}} := \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{d f_1}{d x_p} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_q}{\partial x_1} & \cdots & \frac{d f_q}{d x_p} \end{pmatrix}$$

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Jacobian vs. gradient

- the gradient of a scalar quantity with respect to a parameter vector $\mathbf{w}$ is a column vector of the same size as $\mathbf{w}$
- in contrast, the Jacobian by definition is a row vector
- the following analysis uses Jacobians, so all derivatives we will define are row vectors and need to be transposed
- similarly when a parameter is a matrix W: we need to transpose it so it has the same size as W

chain rule

- if $f : \mathbb{R}^p \to \mathbb{R}^q$ is differentiable at $\mathbf{x}$ and $g : \mathbb{R}^q \to \mathbb{R}^r$ is differentiable at $\mathbf{y} = f(\mathbf{x})$, then $g \circ f : \mathbb{R}^p \to \mathbb{R}^r$ is differentiable at $\mathbf{x}$ and

$$D(g \circ f)(\mathbf{x}) = Dg(\mathbf{y}) \cdot Df(\mathbf{x})$$

  where $\cdot$ denotes matrix multiplication

- how to use it:

$$\frac{\partial \mathbf{z}}{\partial \mathbf{x}_1} = \frac{\partial \mathbf{z}}{\partial \mathbf{x}_2} \cdot \frac{\partial \mathbf{x}_2}{\partial \mathbf{x}_1}$$

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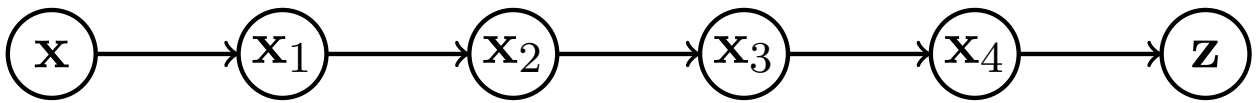

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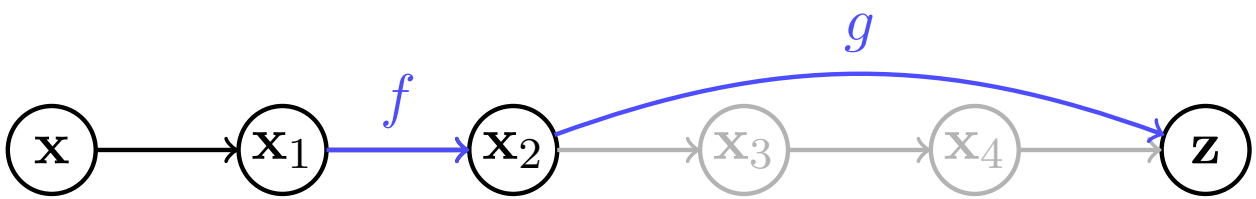

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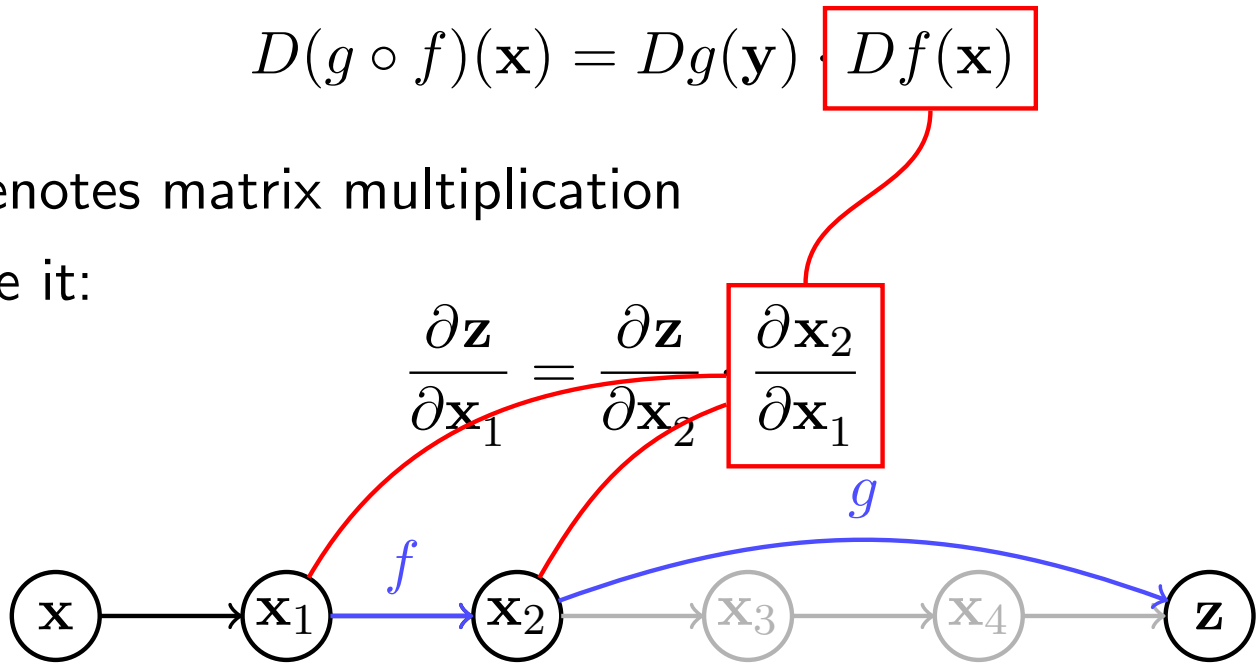

chain rule

- if $f : \mathbb{R}^p \to \mathbb{R}^q$ is differentiable at $\mathbf{x}$ and $g : \mathbb{R}^q \to \mathbb{R}^r$ is differentiable at $\mathbf{y} = f(\mathbf{x})$, then $g \circ f : \mathbb{R}^p \to \mathbb{R}^r$ is differentiable at $\mathbf{x}$ and

$$D(g \circ f)(\mathbf{x}) = Dg(\mathbf{y}) \cdot Df(\mathbf{x})$$

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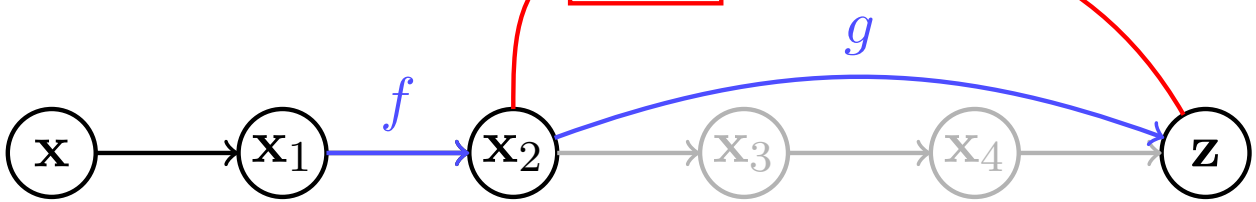

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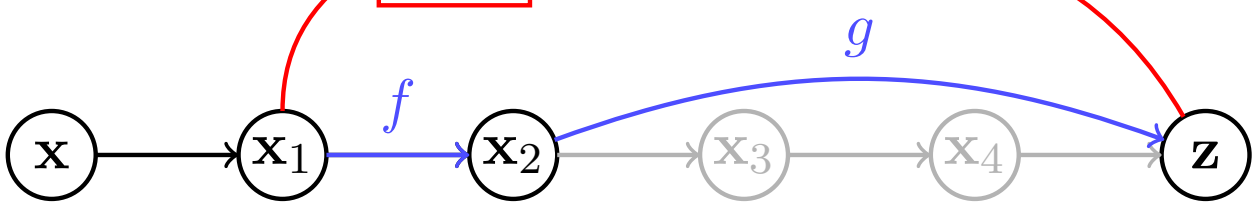

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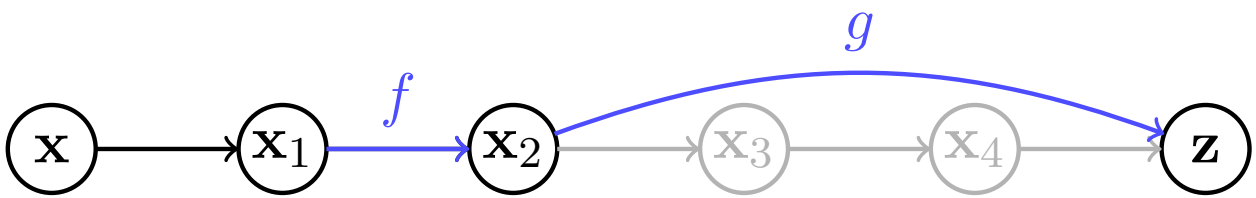

- now, for all i, let us call the partial derivatives

$$d\mathbf{x}_i^\top := \frac{\partial \mathbf{z}}{\partial \mathbf{x}_i}$$

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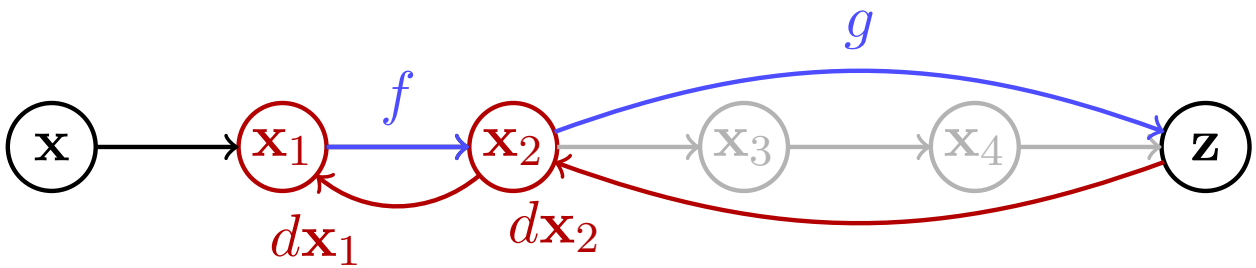
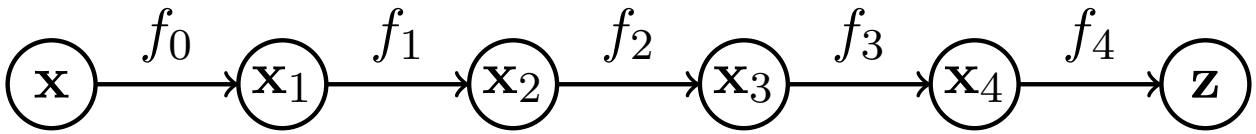


- then, we are back-propagating from $d\mathbf{x}_2$ to $d\mathbf{x}_1$

$$d\mathbf{x}_1^\top = d\mathbf{x}_2^\top \cdot Df(\mathbf{x}_1)$$

chaining

- let $f = f_4 \circ f_3 \circ f_2 \circ f_1 \circ f_0$ and $\mathbf{z} = f(\mathbf{x})$



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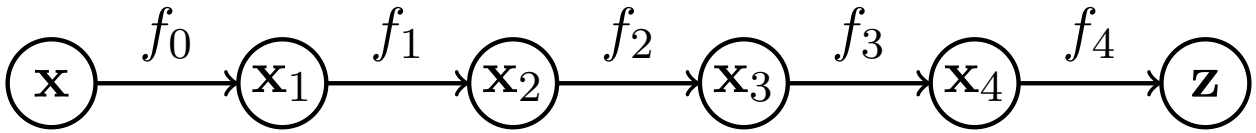

- we apply the chain rule

$$\begin{aligned}
\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = Df(\mathbf{x}) &= D(f_4 \circ f_3 \circ f_2 \circ f_1)(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= D(f_4 \circ f_3 \circ f_2)(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= D(f_4 \circ f_3)(\mathbf{x}_3) \cdot Df_2(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= Df_4(\mathbf{x}_4) \cdot Df_3(\mathbf{x}_3) \cdot Df_2(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_4^\top \cdot Df_3(\mathbf{x}_3) \cdot Df_2(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_3^\top \cdot Df_2(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_2^\top \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_1^\top \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}^\top
\end{aligned}$$

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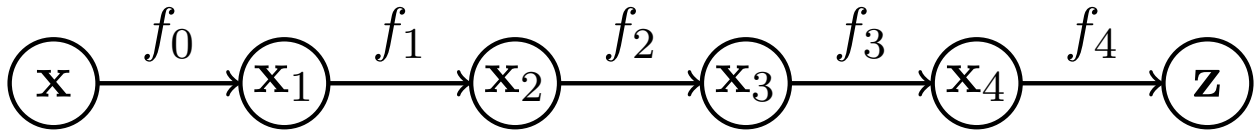

- we apply the chain rule, then collect back into factors $d\mathbf{x}_i$

$$
\begin{aligned}
\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = Df(\mathbf{x}) &= D(f_4 \circ f_3 \circ f_2 \circ f_1)(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
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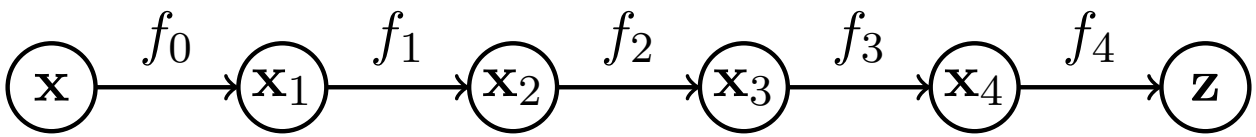
&= Df_4(\mathbf{x}_4) \cdot Df_3(\mathbf{x}_3) \cdot Df_2(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_4^\top \cdot Df_3(\mathbf{x}_3) \cdot Df_2(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_3^\top \cdot Df_2(\mathbf{x}_2) \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_2^\top \cdot Df_1(\mathbf{x}_1) \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}_1^\top \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}^\top
\end{aligned}
$$

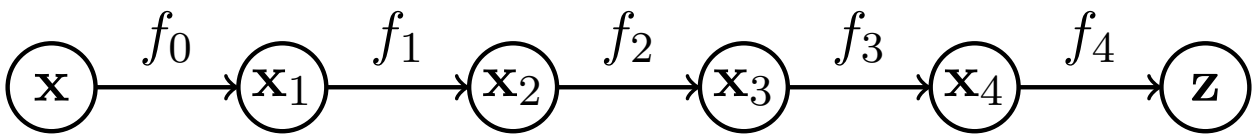
back-propagation



forward pass

$$\mathbf{x}_1 = f_0(\mathbf{x}) \quad \mathbf{x}_2 = f_1(\mathbf{x}_1) \quad \mathbf{x}_3 = f_2(\mathbf{x}_2) \quad \mathbf{x}_4 = f_3(\mathbf{x}_3) \quad \mathbf{z} = f_4(\mathbf{x}_4)$$

back-propagation



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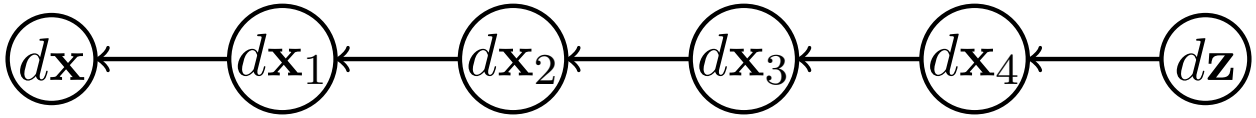

backward pass

$$d\mathbf{z}^\top = I \qquad d\mathbf{x}_4^\top = d\mathbf{z}^\top \cdot Df_4(\mathbf{x}_4) \qquad d\mathbf{x}_3^\top = d\mathbf{x}_4^\top \cdot Df_3(\mathbf{x}_3)$$

$$d\mathbf{x}_2^\top = d\mathbf{x}_3^\top \cdot Df_3(\mathbf{x}_3) \qquad d\mathbf{x}_1^\top = d\mathbf{x}_2^\top \cdot Df_1(\mathbf{x}_1) \qquad d\mathbf{x}^\top = d\mathbf{x}_1^\top \cdot Df_0(\mathbf{x})$$

back-propagation is dynamic programming

- we need to store all the $\mathbf{x}_i$ that we compute in the forward pass before the backward pass begins
- the $d\mathbf{x}_i$ can be computed on the fly in reverse order on a chain, but may need to be all stored on a general network structure
- that's exactly what we do in dynamic programming: break the problem down into a collection of smaller, overlapping subproblems, store their solutions and save computation time at the expense of a (hopefully) modest expenditure in storage space
- as in all dynamic programming problems, there is a bottom-up approach that we have just described, and a top-down approach coming out of the recursive formulation through memoization; this can be useful if we are looking for the derivative with respect to only few parameters

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partial derivatives

- in the following, for any vector $\mathbf{x}$ appearing in our function, we will use the symbol

$$d\mathbf{x}^\top := \frac{\partial}{\partial \mathbf{x}}$$

  for the partial derivative operator of any quantity with respect to $\mathbf{x}$
- in practice, we will apply this to the quantity we want to optimize, *i.e.* the error
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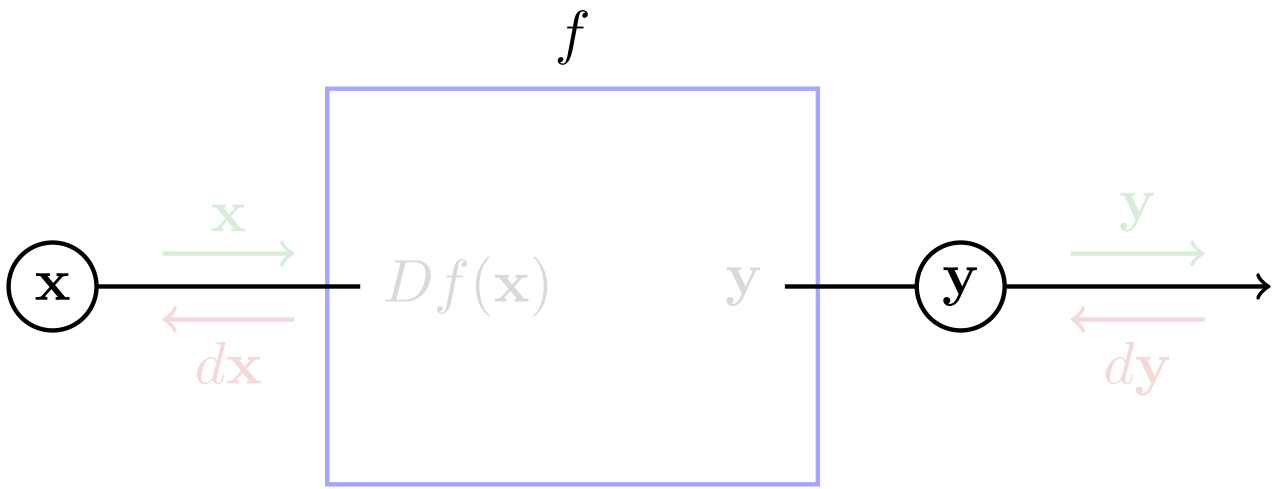
nodes



- to every variable $\mathbf{y}$ is associated a node with the function f that produces it, from input variable $\mathbf{x}$
- given $\mathbf{x}$, derivative $Df(\mathbf{x})$ is "stored", and output $\mathbf{y}$ is computed and flows forward
- given $d\mathbf{y}$, partial derivative $d\mathbf{x}$ is computed and flows backward

$$d\mathbf{x}^\top = d\mathbf{y}^\top \cdot Df(\mathbf{x}) \quad \text{or} \quad \frac{\partial}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{y}} \cdot \frac{\partial \mathbf{y}}{\partial \mathbf{x}}$$

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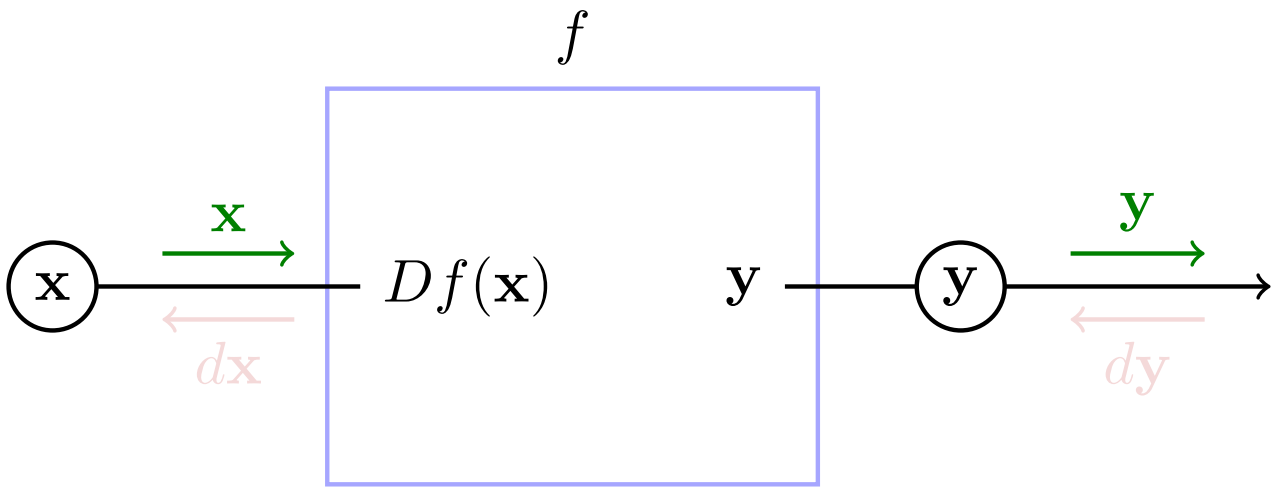

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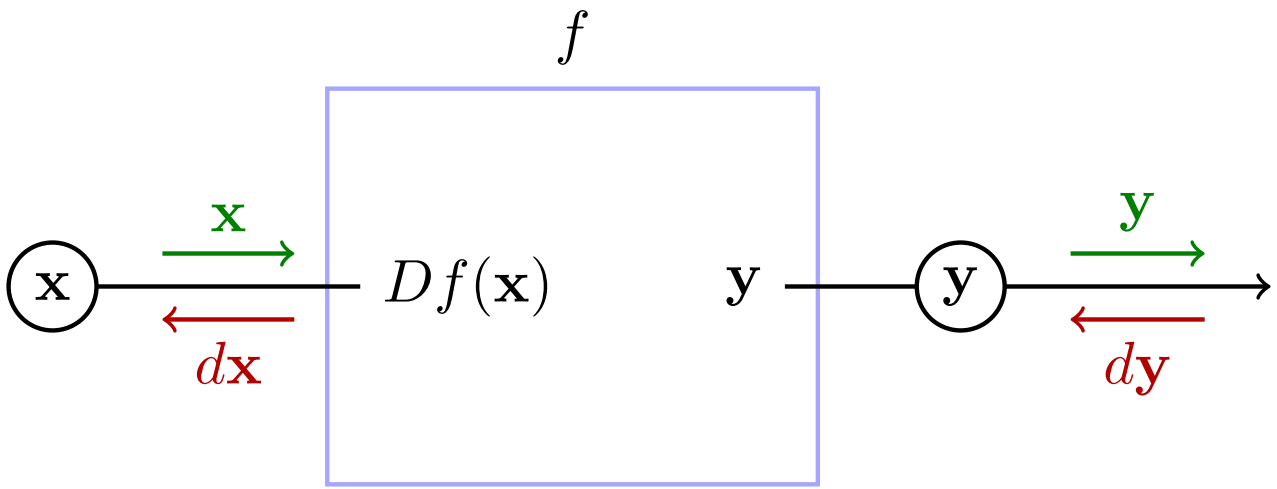

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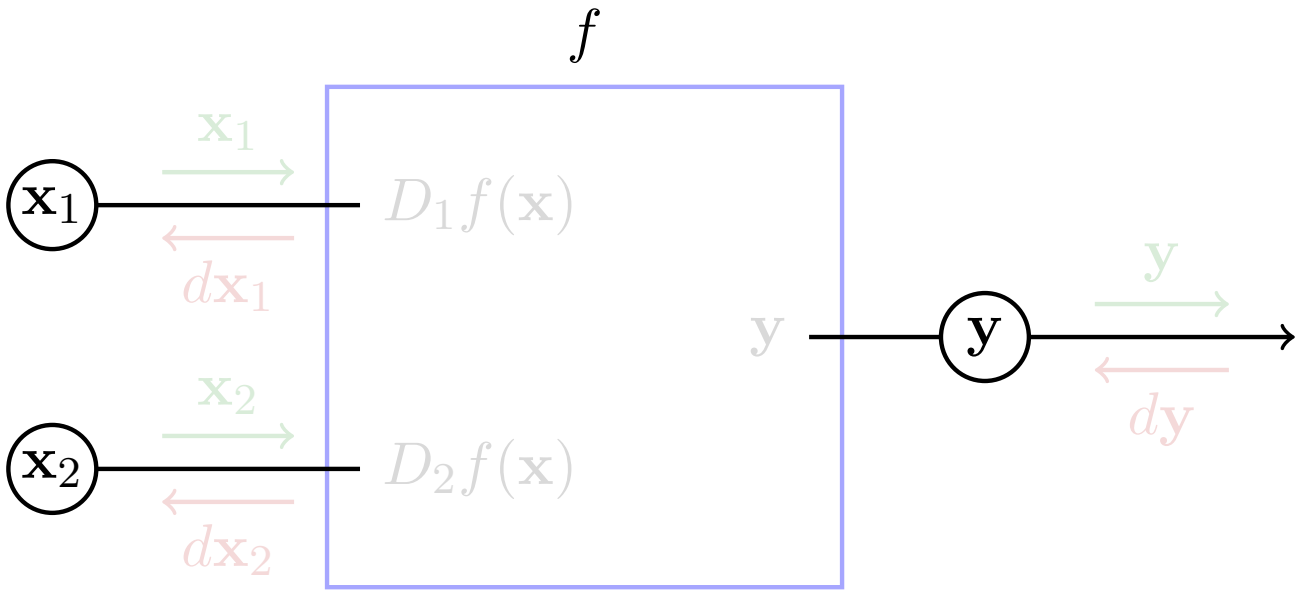
splitting the input



- we split input vector $\mathbf{x}$ into subvectors as $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$
- then, the derivative consists of blocks stacked horizontally

$$Df(\mathbf{x}) = (D_1 f \;\; D_2 f)(\mathbf{x}) \quad \text{or} \quad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial \mathbf{y}}{\partial \mathbf{x}_1} & \frac{\partial \mathbf{y}}{\partial \mathbf{x}_2} \end{pmatrix}$$

- $d\mathbf{x}$ is also split as $d\mathbf{x} = (d\mathbf{x}_1, d\mathbf{x}_2)$ and $d\mathbf{x} = d\mathbf{y} \cdot Df(\mathbf{x})$ becomes

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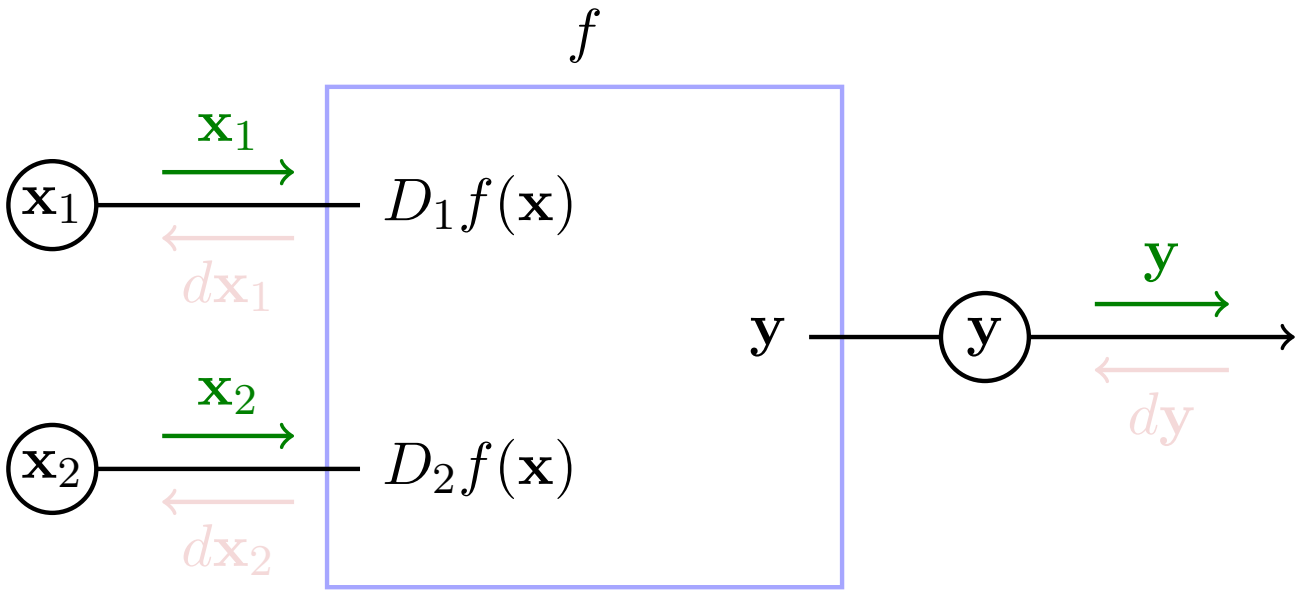

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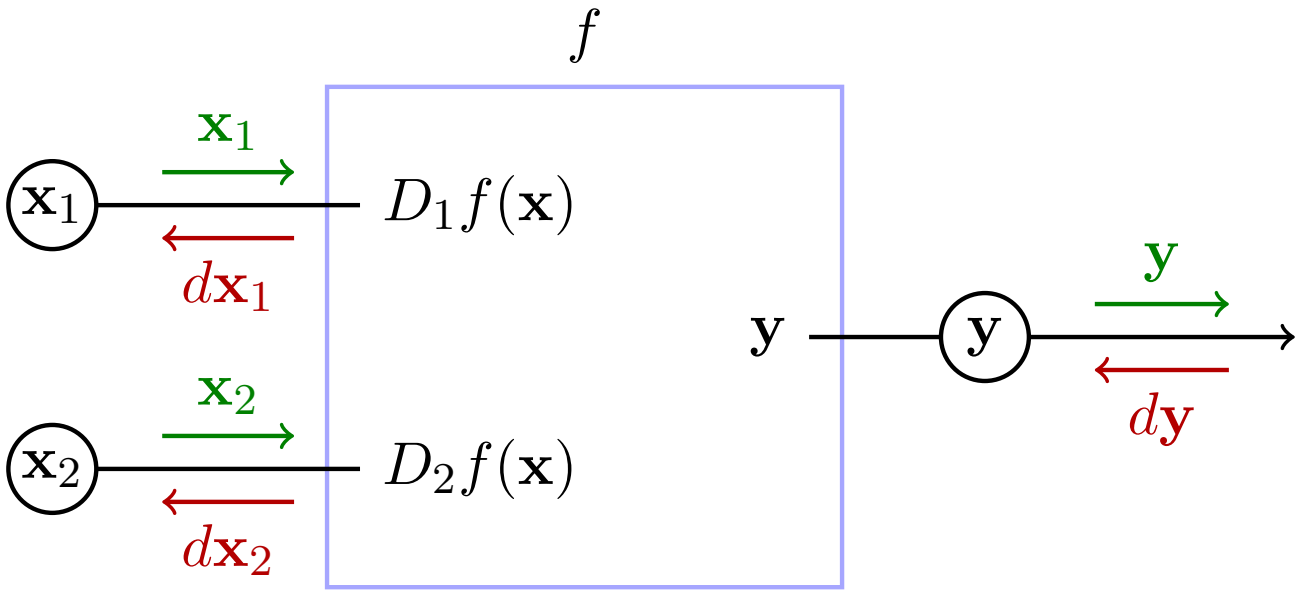

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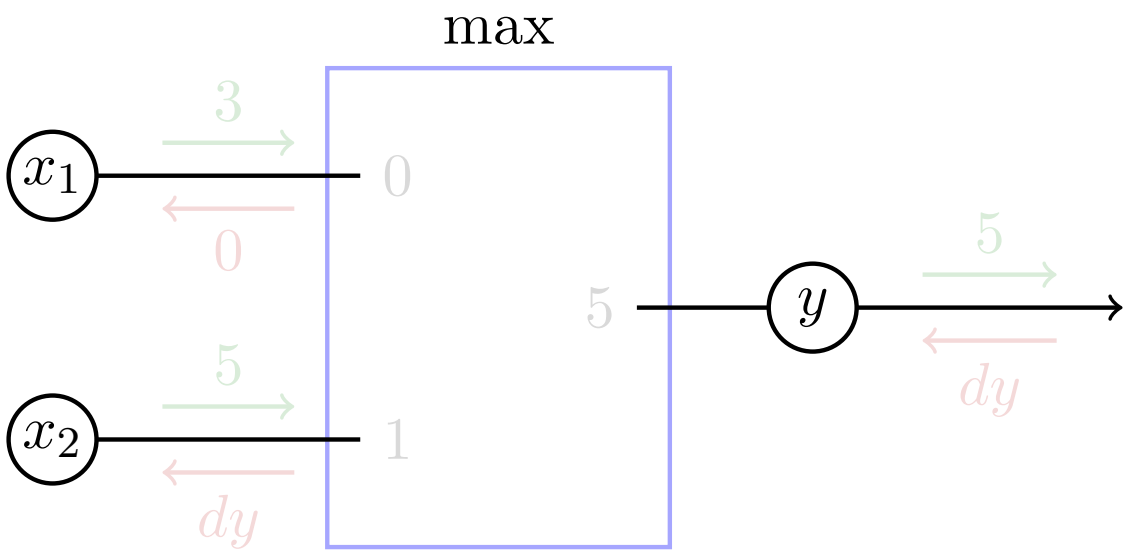
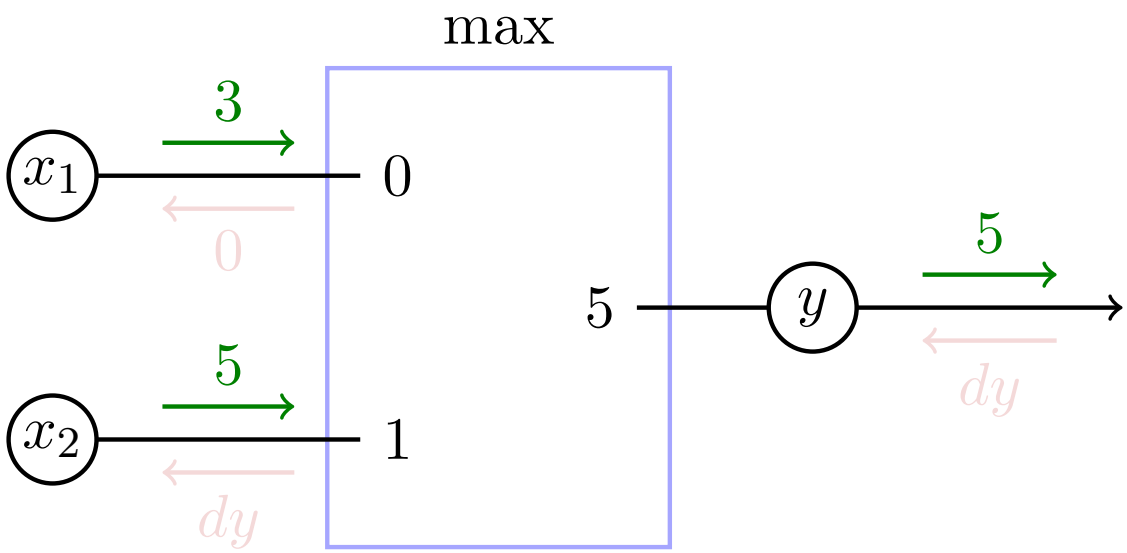
example: maximum



- if $f(x_1, x_2) = \max(x_1, x_2)$, then $D_i f(x_1, x_2) = \mathbb{1}[x_i = \max(x_1, x_2)]$
- and dy is routed into the branch of the maximum input

example: maximum



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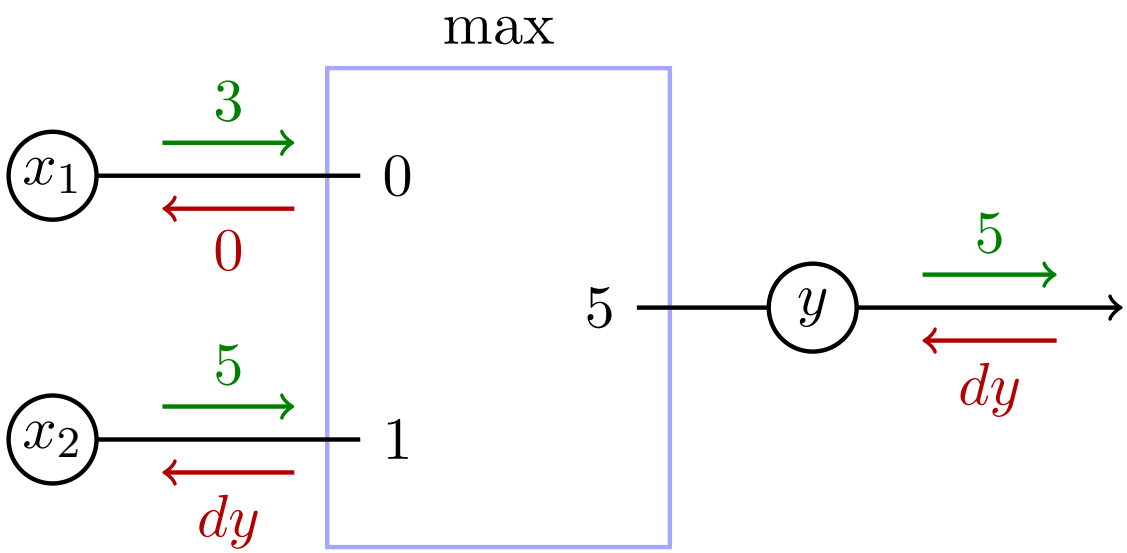

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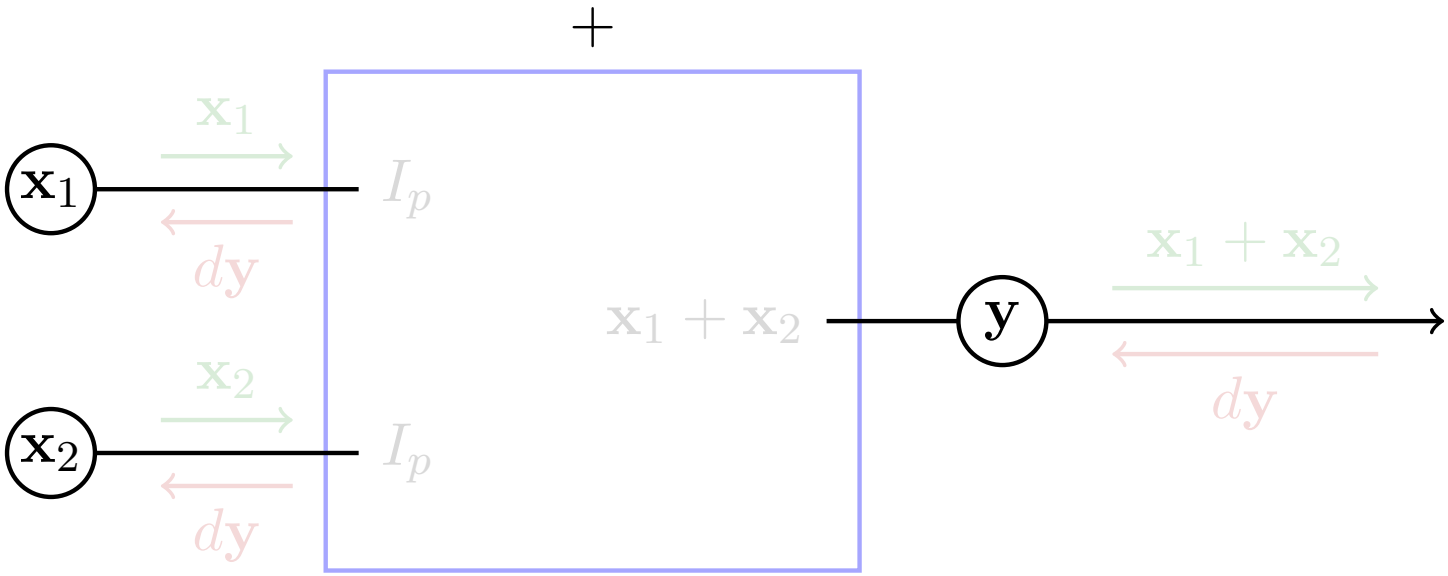
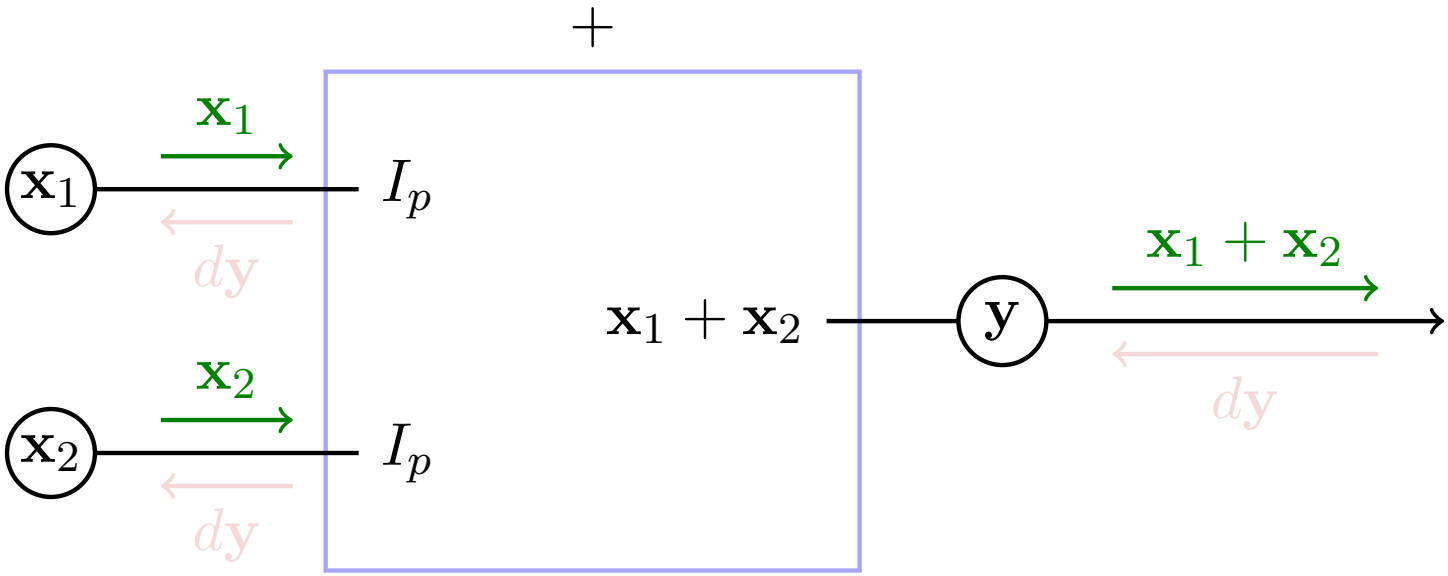
example: sum



- if $f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1 + \mathbf{x}_2$ and $\mathbf{x}_i \in \mathbb{R}^p$, then $D_i f(\mathbf{x}_1, \mathbf{x}_2) = I_p$
- and $d\mathbf{y}$ is distributed to both branches

example: sum



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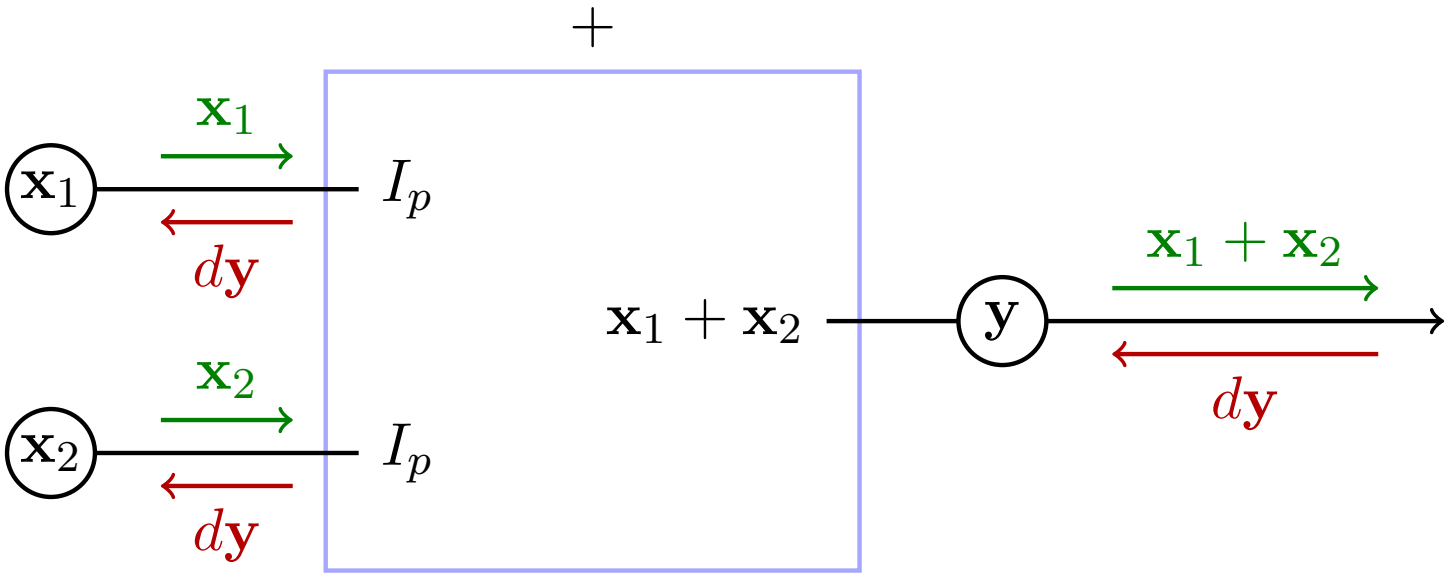
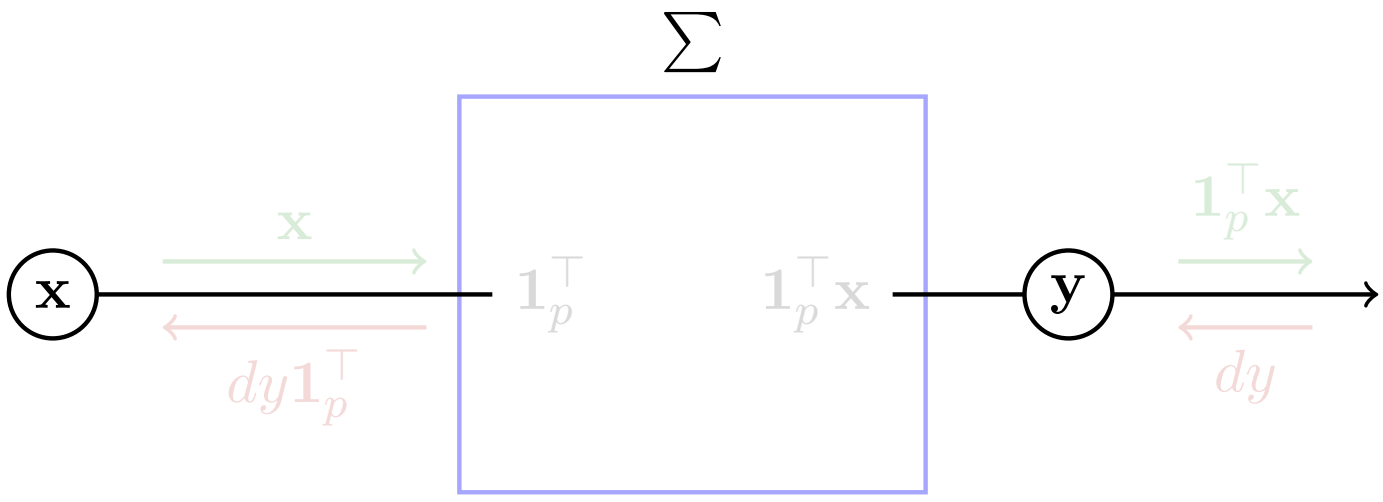
example: sum



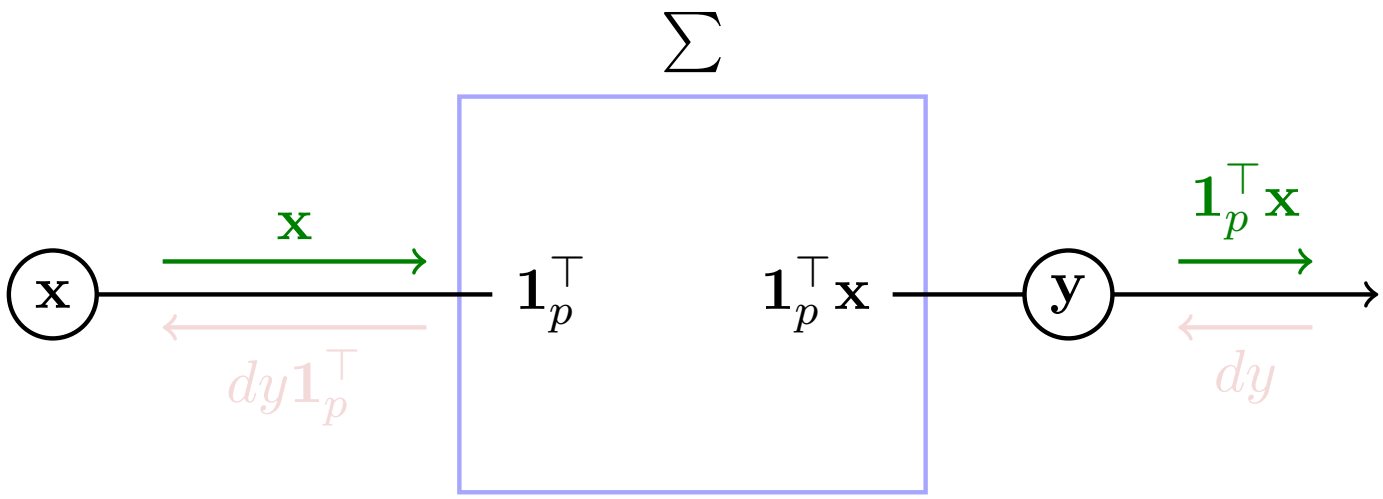
- if $f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1 + \mathbf{x}_2$ and $\mathbf{x}_i \in \mathbb{R}^p$, then $D_i f(\mathbf{x}_1, \mathbf{x}_2) = I_p$
- and $d\mathbf{y}$ is distributed to both branches

example: vector sum



- if $f(\mathbf{x}) = \mathbf{1}_p^\top \mathbf{x} = \sum_{i=1}^p x_i$ and $\mathbf{x} \in \mathbb{R}^p$, then $Df(\mathbf{x}) = \mathbf{1}_p^\top$
- and dy is distributed to every element

example: vector sum



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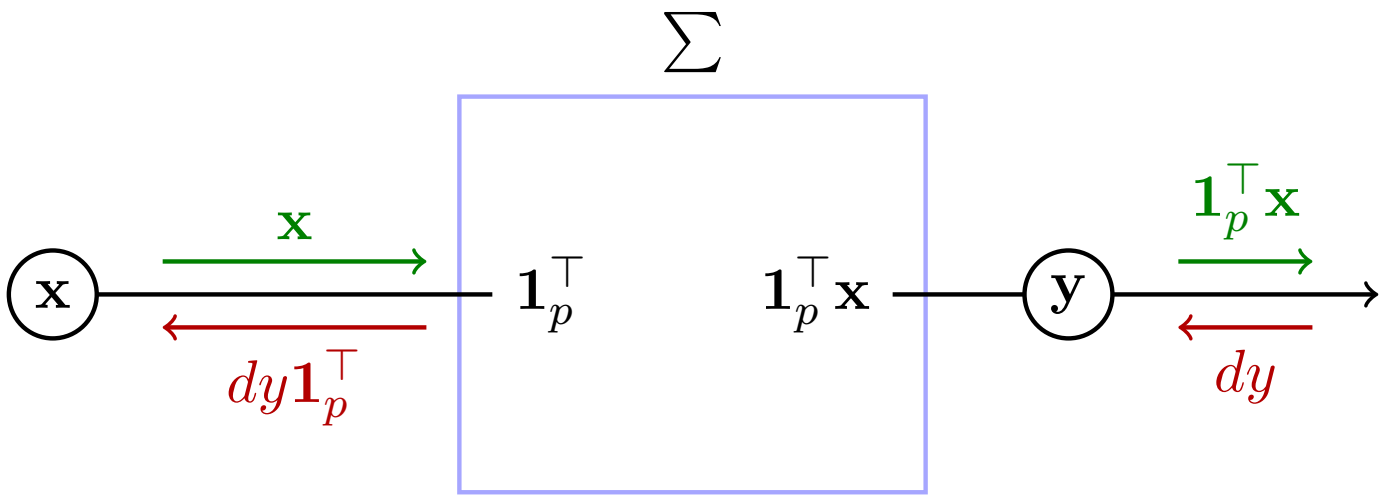

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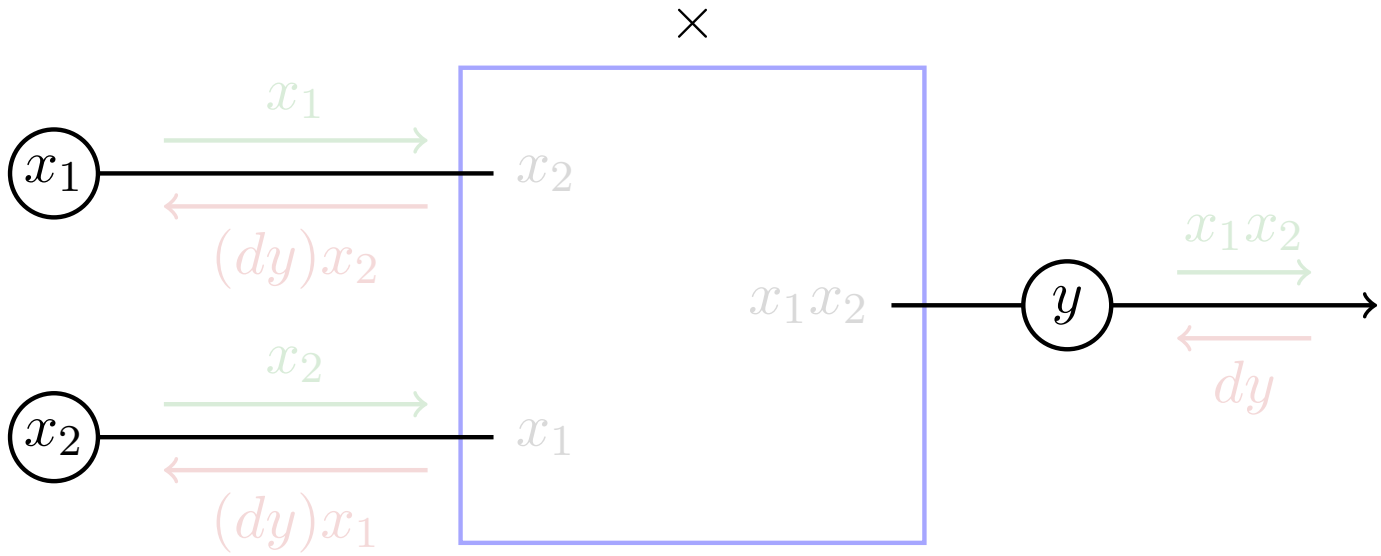
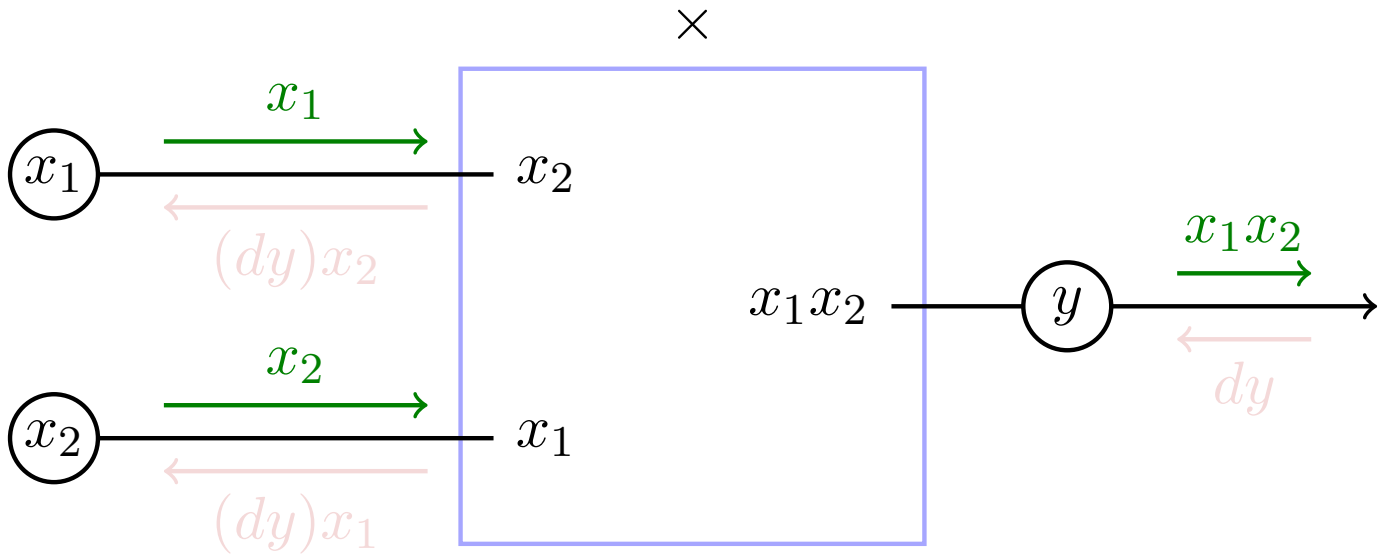
example: product



- if $f(x_1, x_2) = x_1x_2$, then $D_1f(x_1, x_2) = x_2$ and $D_2f(x_1, x_2) = x_1$
- the derivative on each branch is multiplied by the input of the other

example: product



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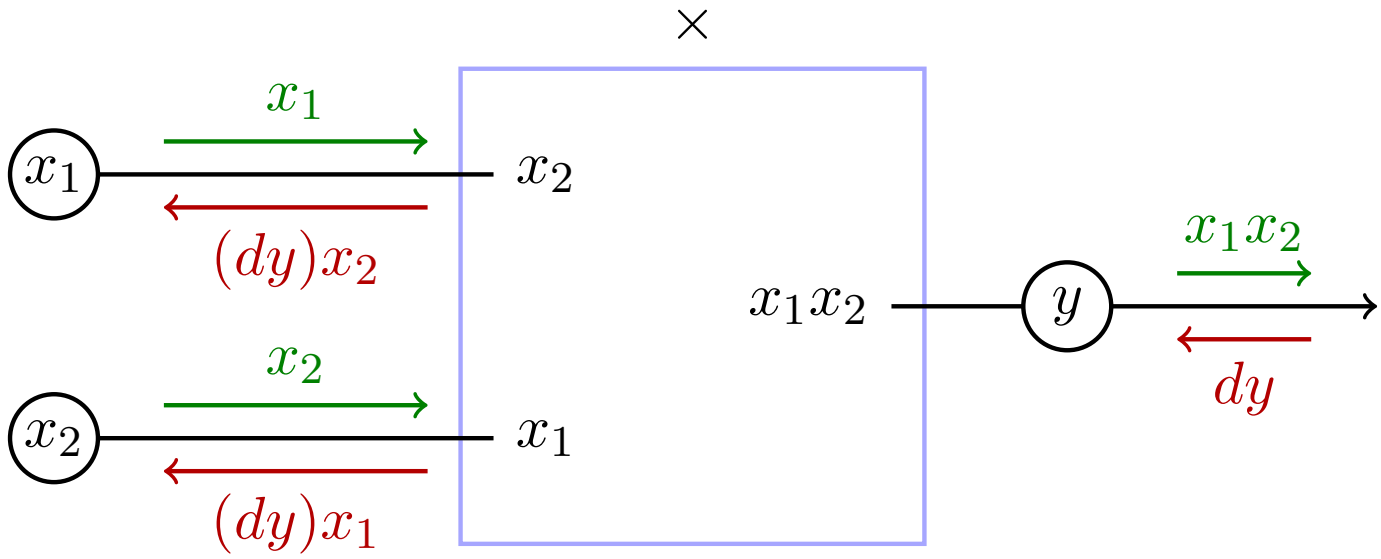

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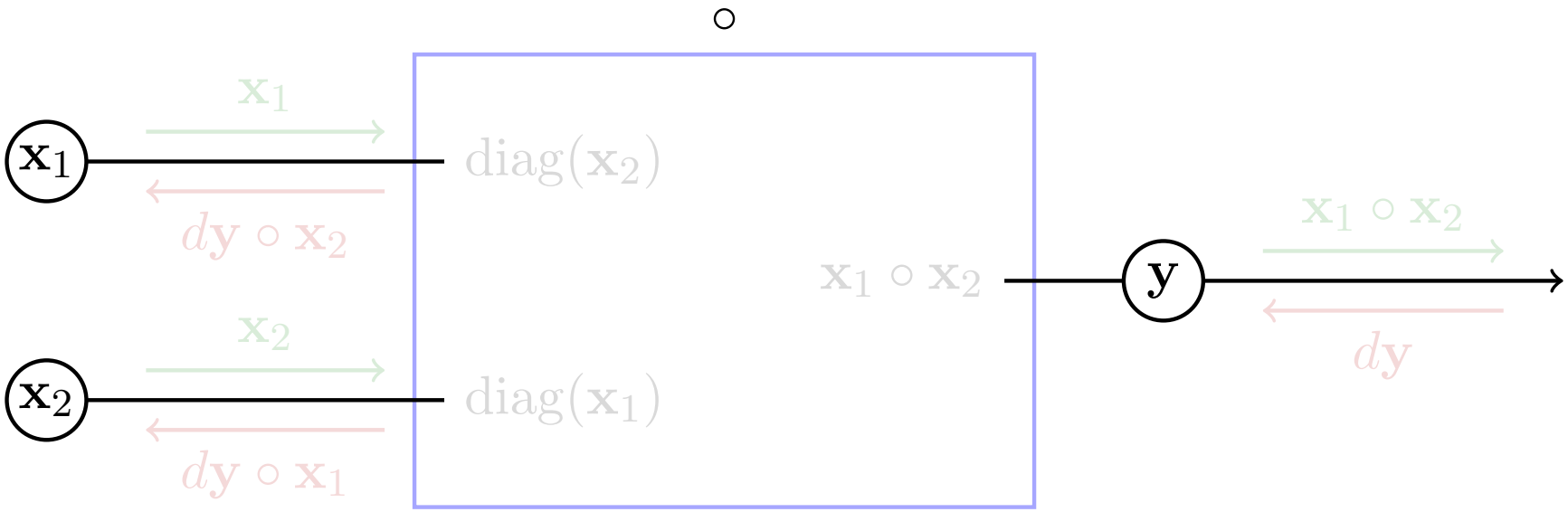
example: Hadamard (element-wise) product



- if $f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1 \circ \mathbf{x}_2$, then $D_1 f(\mathbf{x}_1, \mathbf{x}_2) = \mathrm{diag}(\mathbf{x}_2)$ and $D_2 f(\mathbf{x}_1, \mathbf{x}_2) = \mathrm{diag}(\mathbf{x}_1)$
- the derivative on each branch is element-wise multiplied by the input of the other

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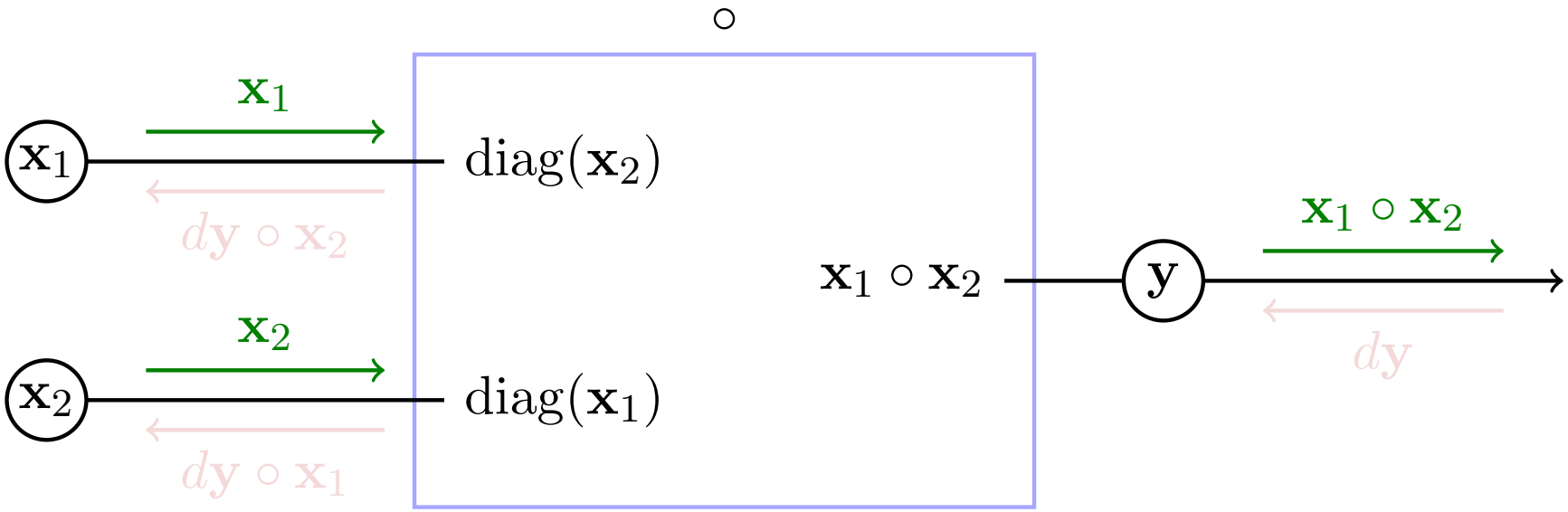

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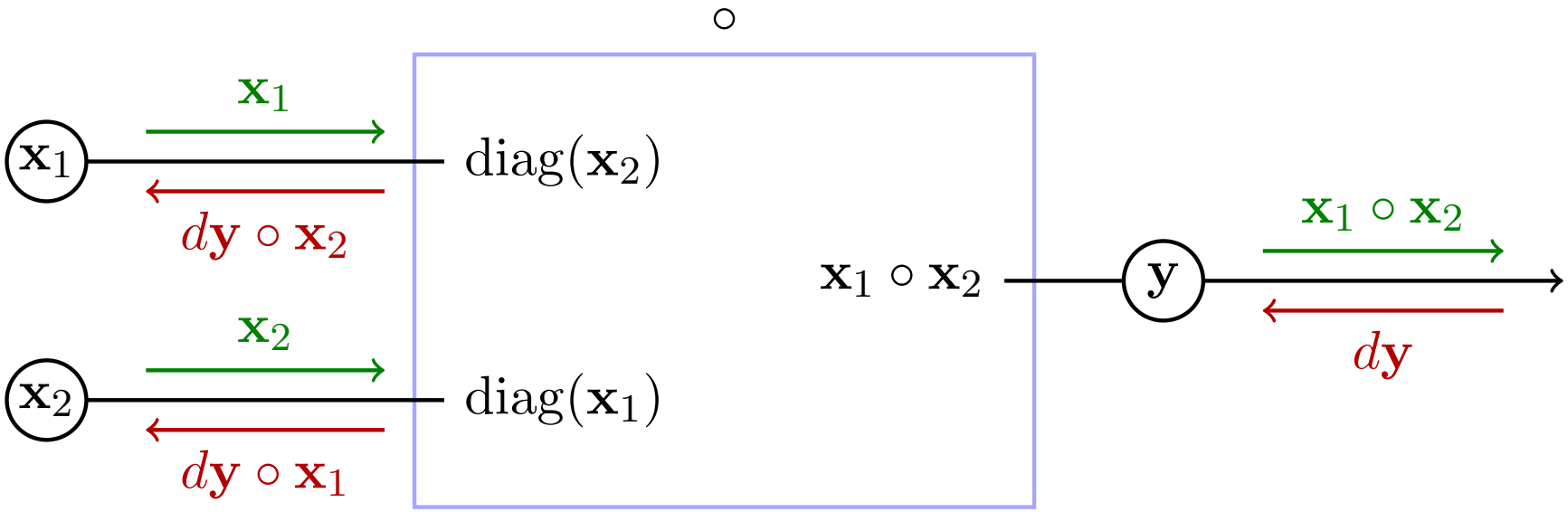

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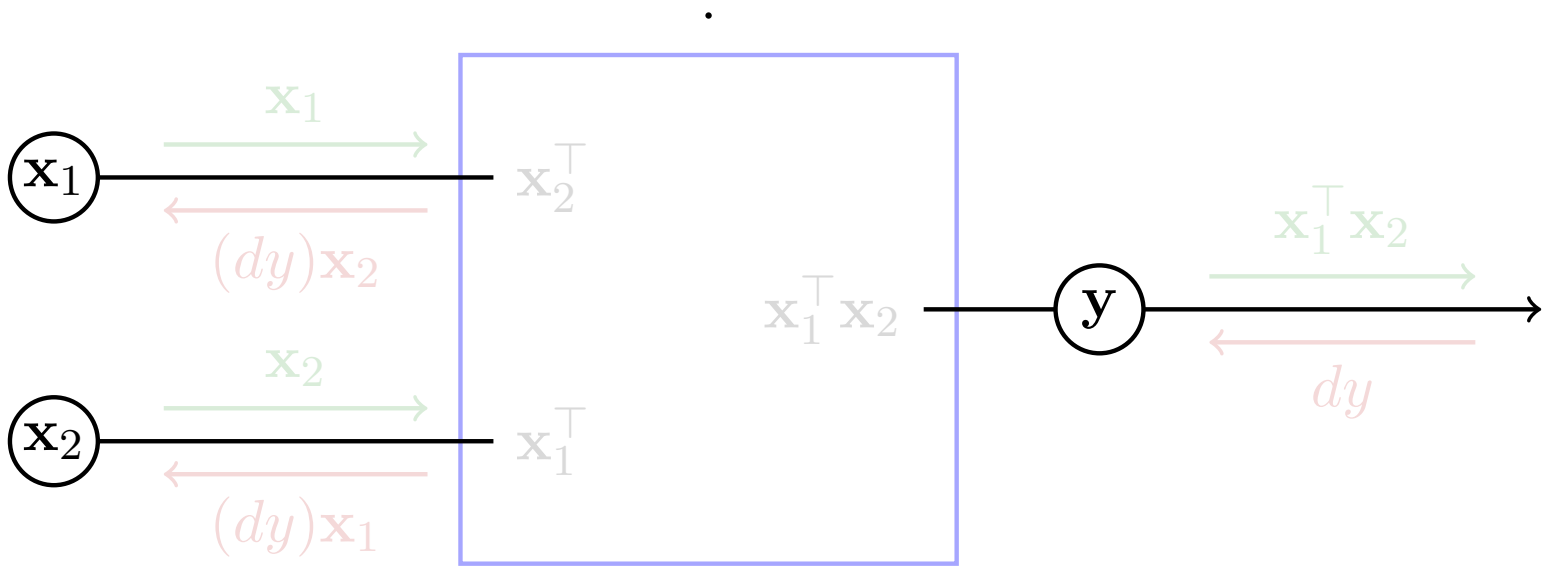
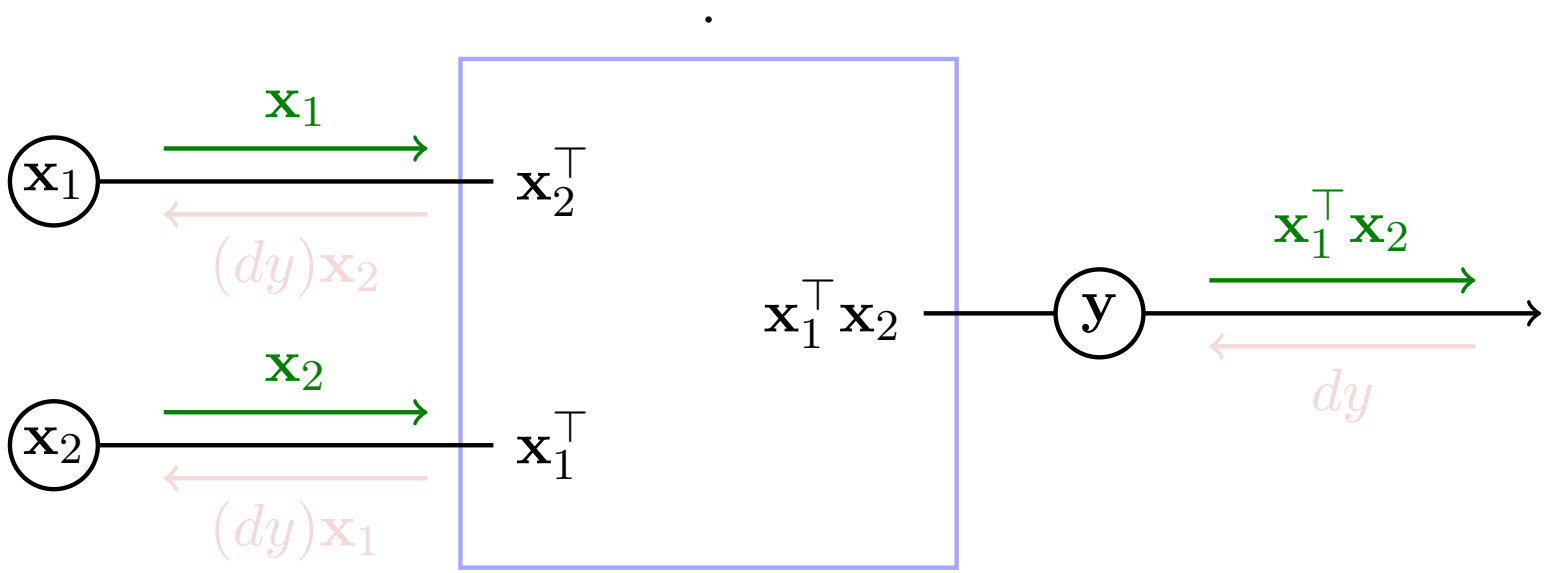
example: dot product



- if $f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1 \cdot \mathbf{x}_2 = \mathbf{x}_1^\top \mathbf{x}_2$, then $D_1 f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_2$ and $D_2 f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1$
- the derivative on each branch is multiplied by the input of the other; this can be seen by composing an element-wise product with a vector sum

example: dot product



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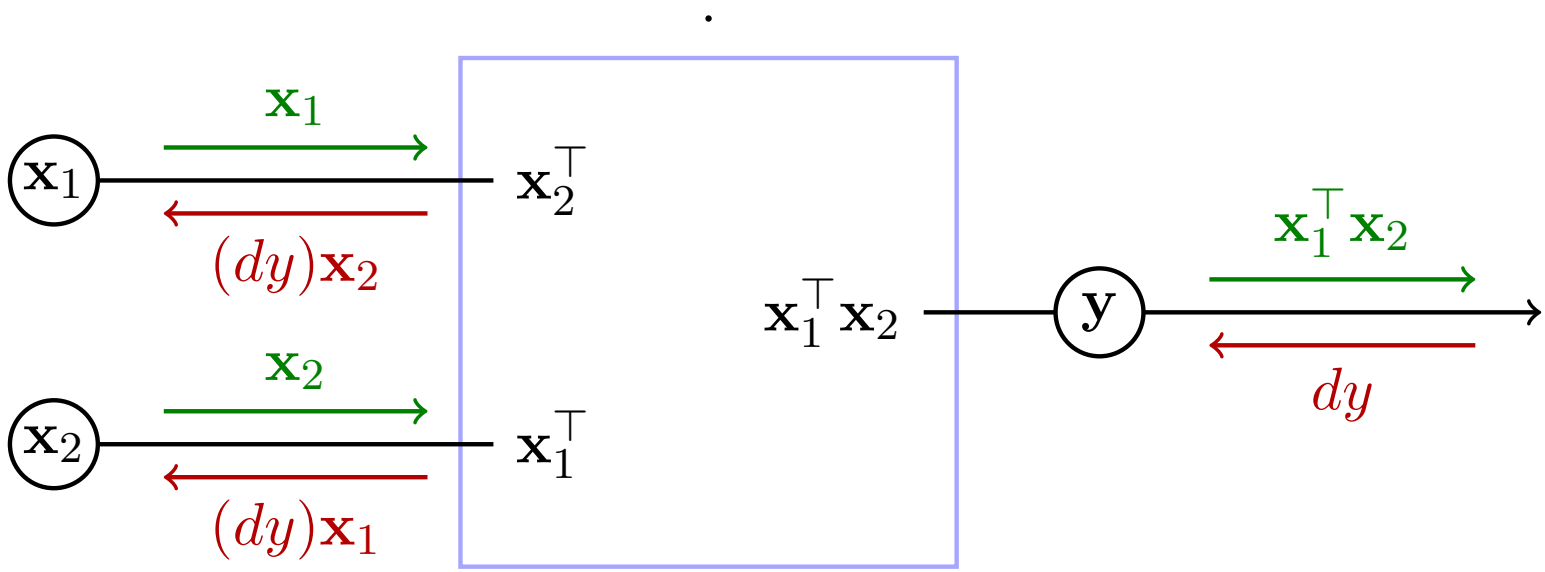
example: dot product



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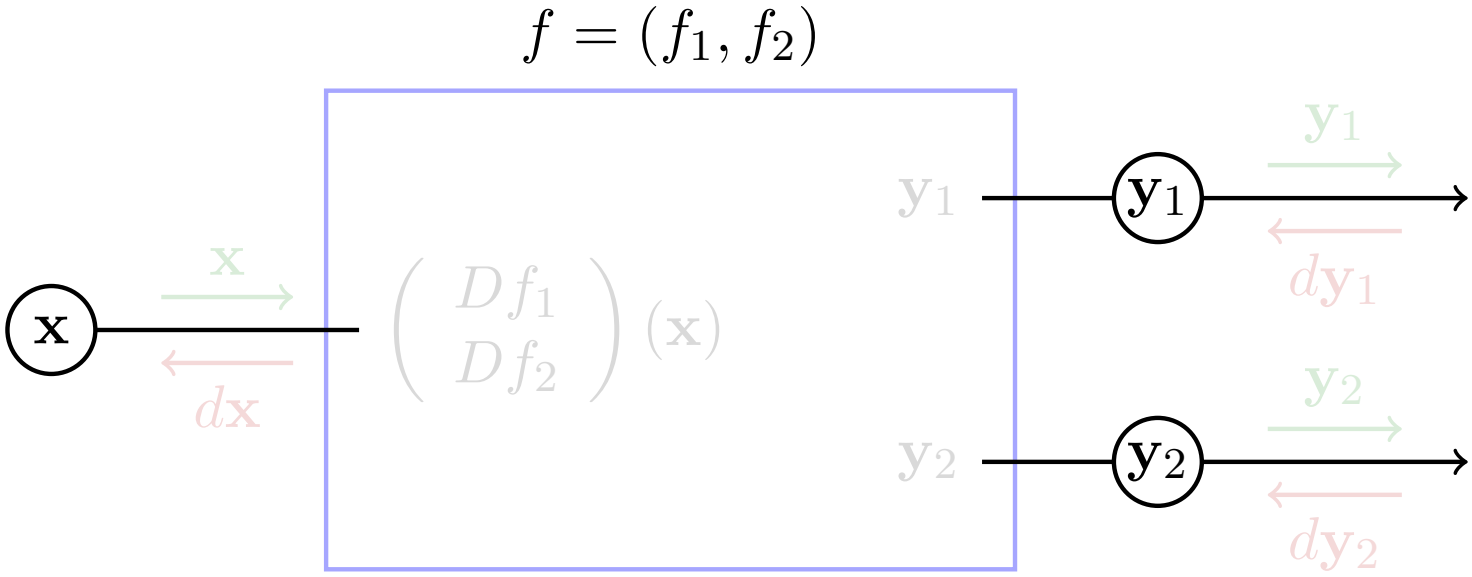
splitting the output



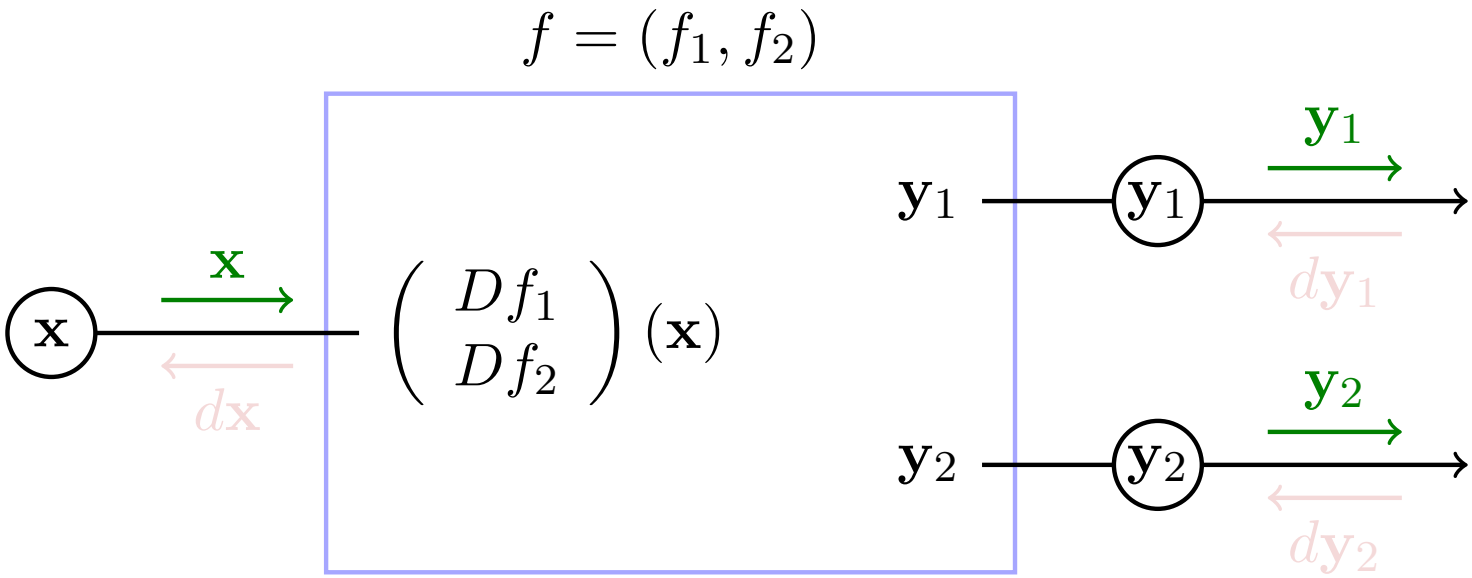
- we split output $\mathbf{y}$ into subvectors as $\mathbf{y} = (\mathbf{y}_1, \mathbf{y}_2) = (f_1(\mathbf{x}), f_2(\mathbf{x}))$
- then, the derivative consists of blocks stacked vertically

$$Df(\mathbf{x}) = (Df_1; Df_2)(\mathbf{x}) \quad \text{or} \quad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \left(\frac{\partial \mathbf{y}_1}{\partial \mathbf{x}}; \frac{\partial \mathbf{y}_2}{\partial \mathbf{x}} \right)$$

- $d\mathbf{y}$ is also split as $d\mathbf{y} = (d\mathbf{y}_1, d\mathbf{y}_2)$ and $d\mathbf{x} = d\mathbf{y} \cdot Df(\mathbf{x})$ becomes

$$d\mathbf{x}^\top = \sum_i d\mathbf{y}_i^\top \cdot Df_i(\mathbf{x}) \quad \text{or} \quad \frac{\partial}{\partial \mathbf{x}} = \sum_i \frac{\partial}{\partial \mathbf{y}_i} \cdot \frac{\partial \mathbf{y}_i}{\partial \mathbf{x}}$$

splitting the output



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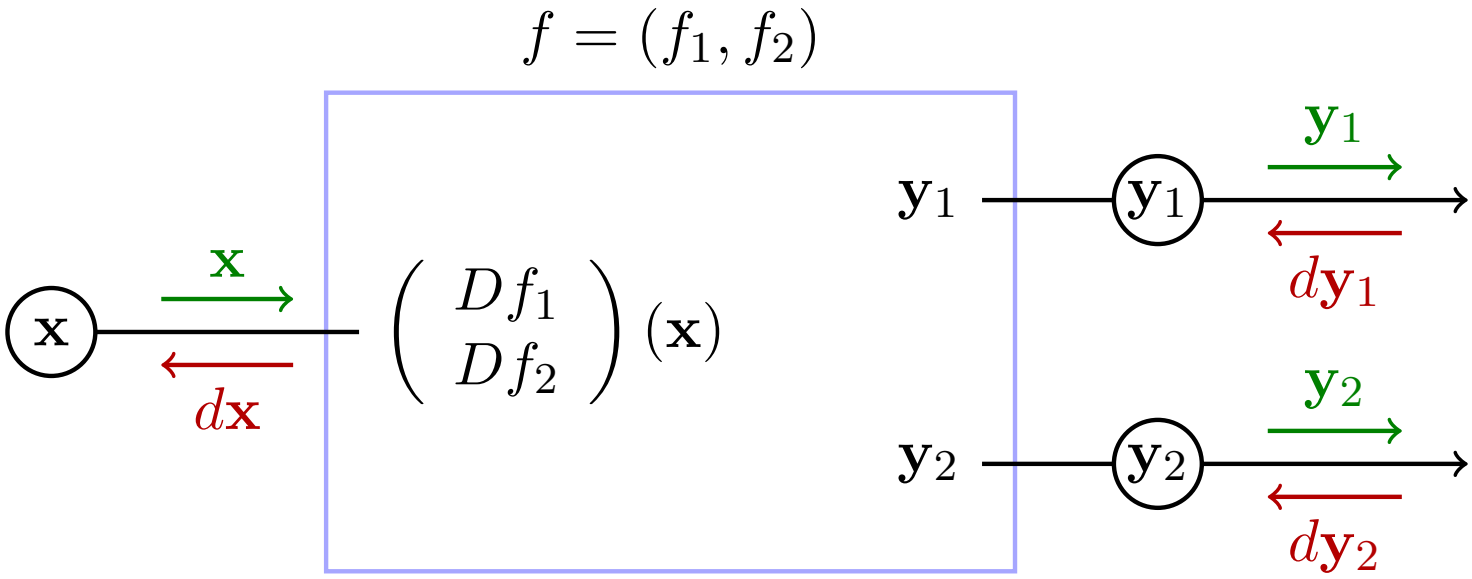

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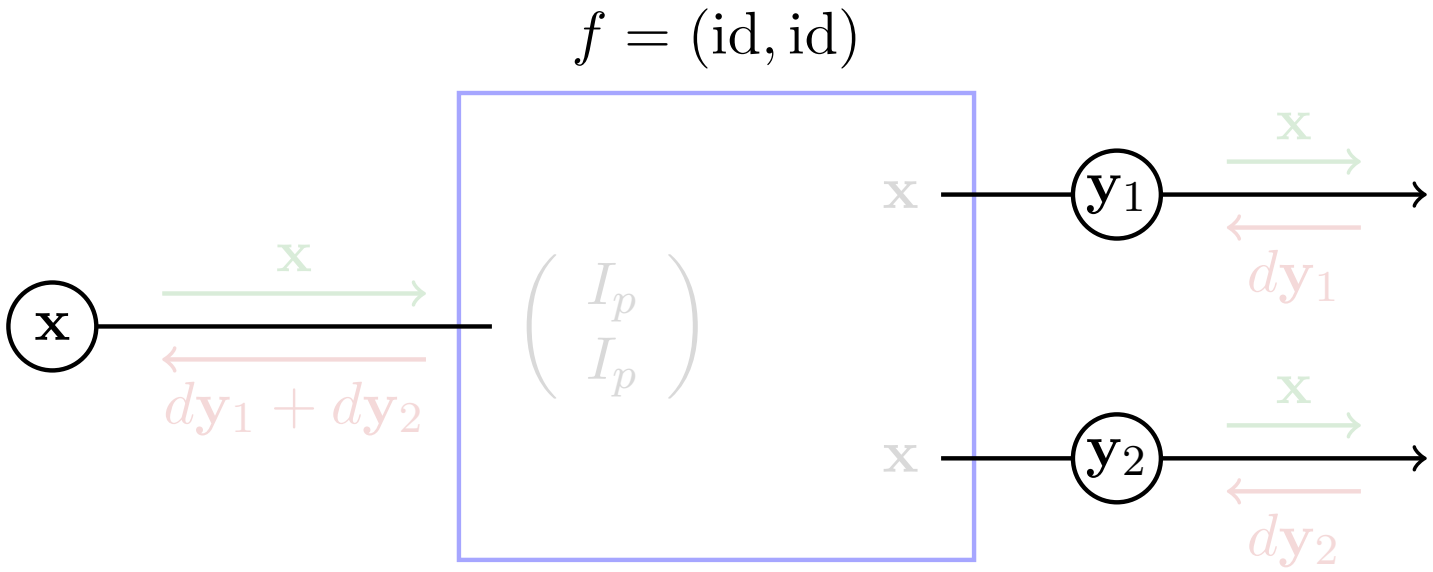
example: splitter (sharing)

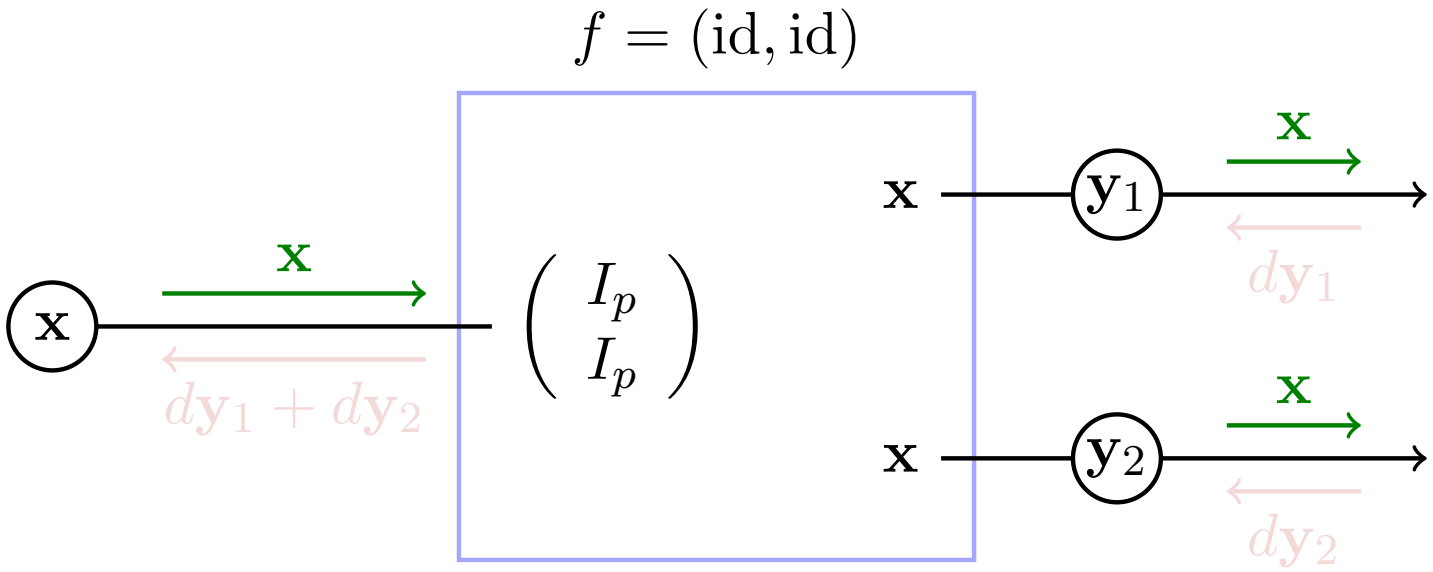


- if $f(\mathbf{x}) = (\mathbf{x}, \mathbf{x})$ and $\mathbf{x} \in \mathbb{R}^p$, then $Df(\mathbf{x}) = (I_p; I_p)$
- and the node behaves like sum backwards

$$d\mathbf{x} = d\mathbf{y}_1 + d\mathbf{y}_2 \quad \text{or} \quad \frac{\partial}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{y}_1} + \frac{\partial}{\partial \mathbf{y}_2}$$

- whenever a variable is shared (used more than once), we need to sum the gradients flowing from all paths where it appears

example: splitter (sharing)



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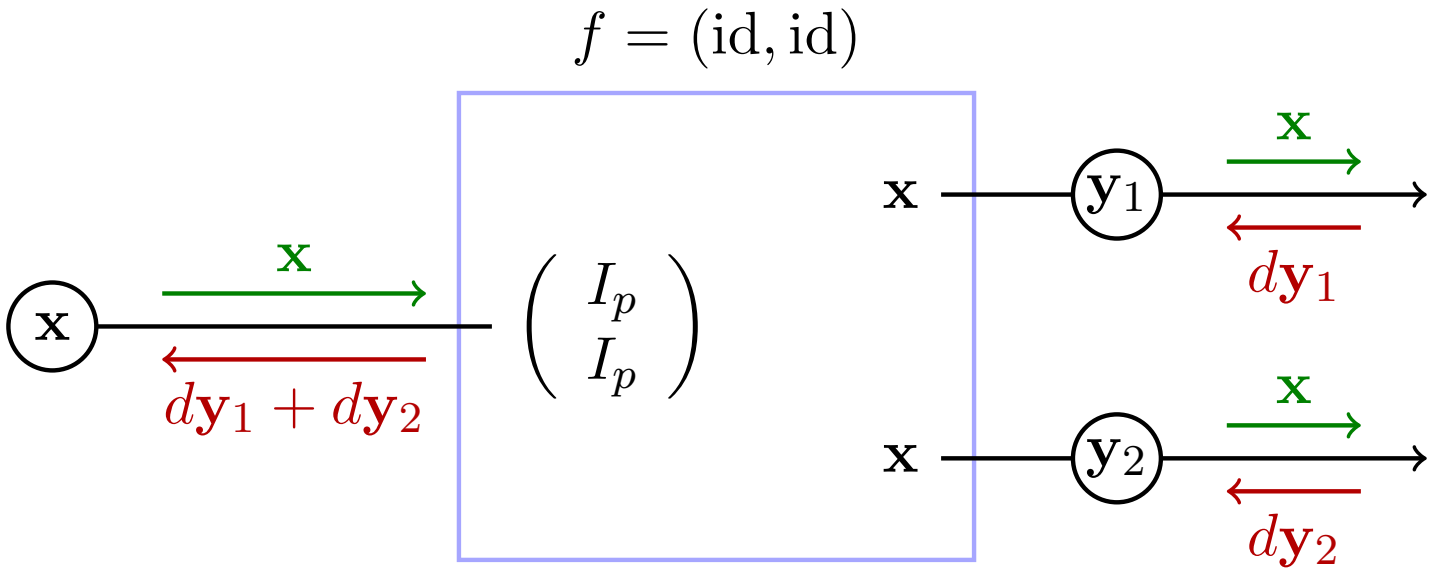

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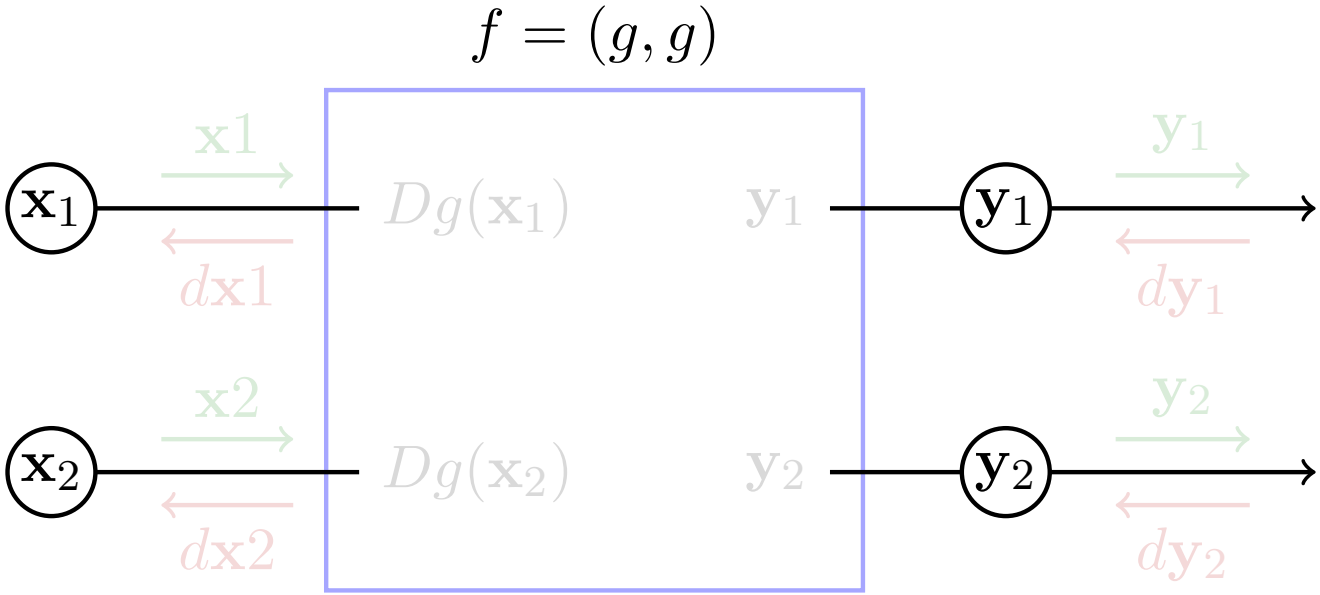
example: tuples



- if $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$, $\mathbf{y} = (\mathbf{y}_1, \mathbf{y}_2)$ and $f = (g, g)$, then $Df(\mathbf{x})$ is block-wise diagonal: $\mathrm{diag}(Dg(\mathbf{x}_1), Dg(\mathbf{x}_2))$
- and the backward paths flow independently like the forward

$$d\mathbf{x}_i^\top = d\mathbf{y}_i^\top \cdot Dg(\mathbf{x}_i) \quad \text{or} \quad \frac{\partial}{\partial \mathbf{x}_i} = \frac{\partial}{\partial \mathbf{y}_i} \cdot \frac{\partial \mathbf{y}_i}{\partial \mathbf{x}_i}$$

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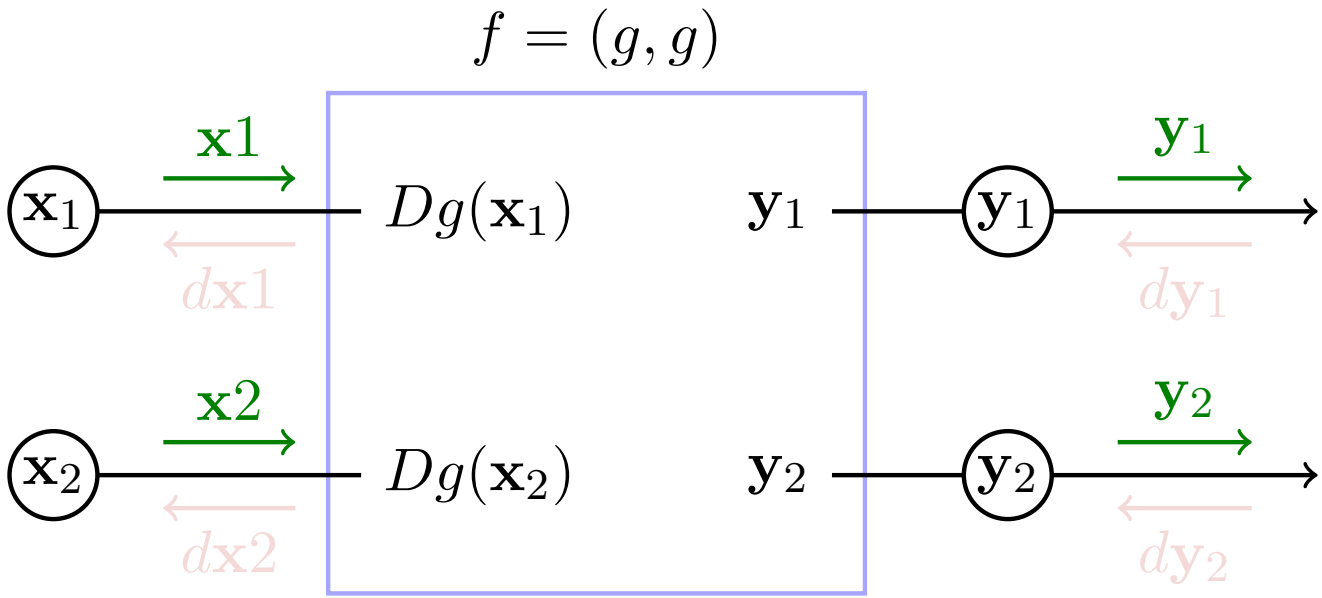

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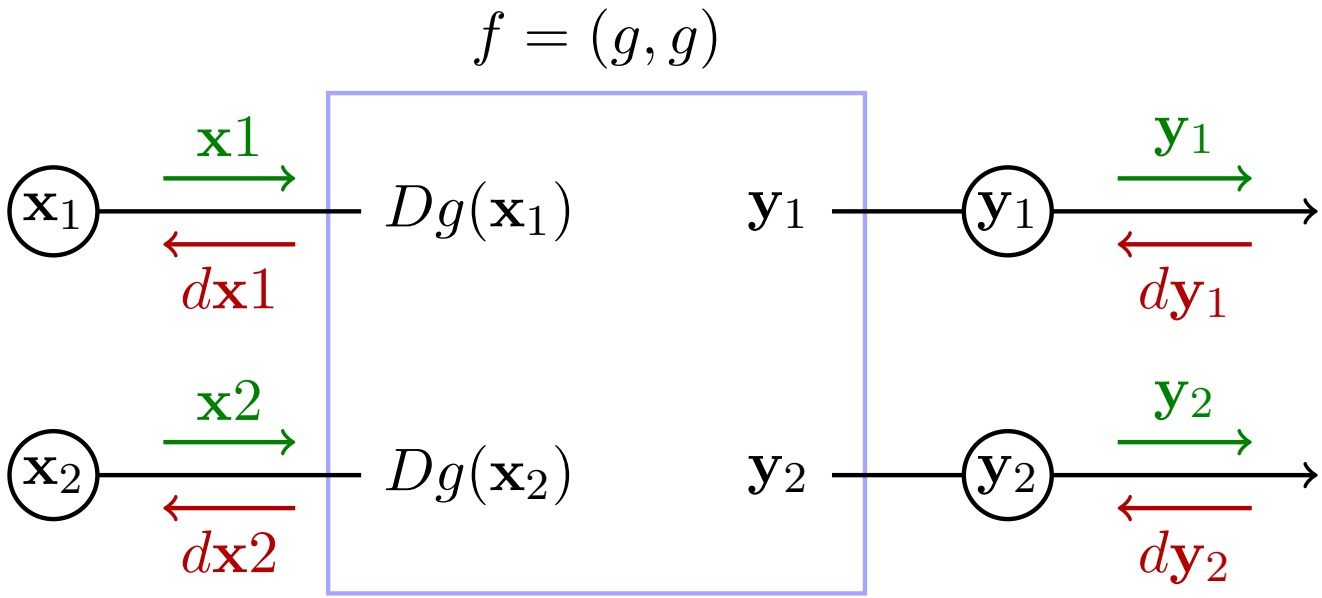

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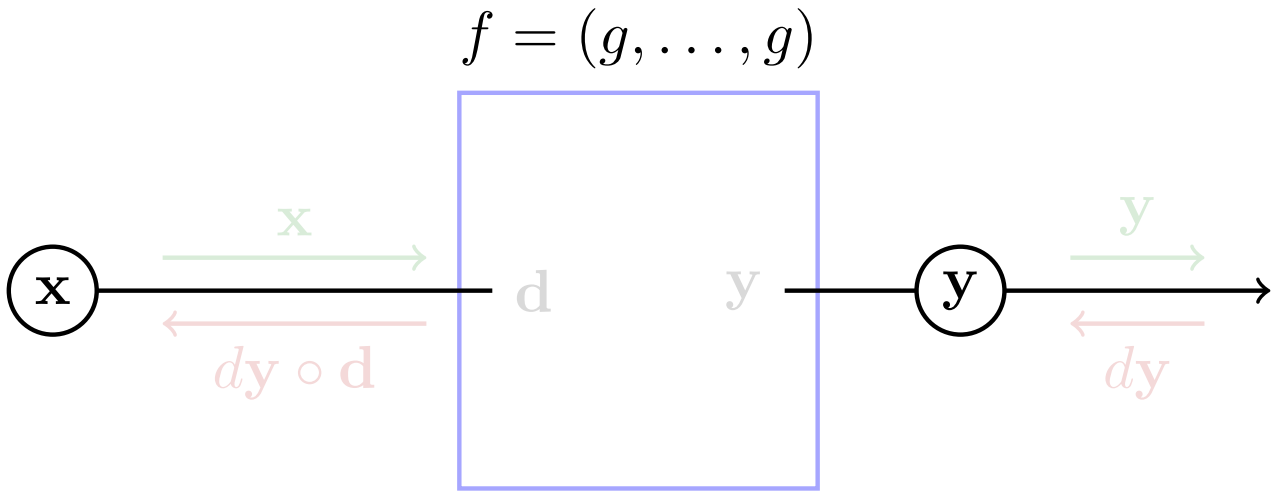
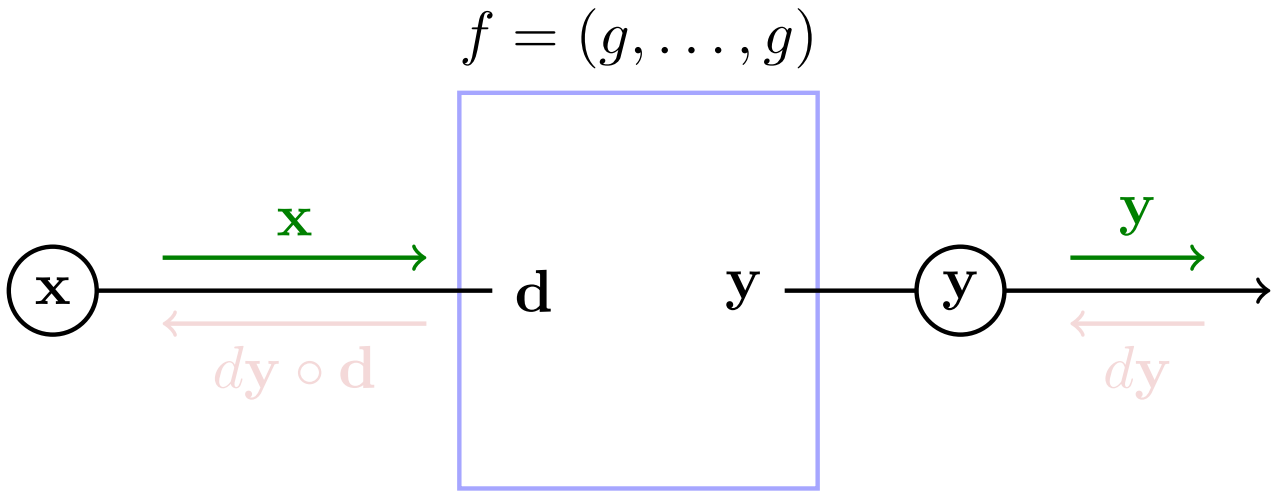
example: element-wise functions



- if $\mathbf{x} \in \mathbb{R}^p$ and f is element-wise with $f(\mathbf{x}) = (g(x_1), \ldots, g(x_p))$ where $g : \mathbb{R} \to \mathbb{R}$, then $Df(\mathbf{x}) = \operatorname{diag} \mathbf{d}$ is diagonal, where $\mathbf{d} = (Dg(x_1), \ldots, Dg(x_p))$
- and the partial derivatives are element-wise multiplied

example: element-wise functions



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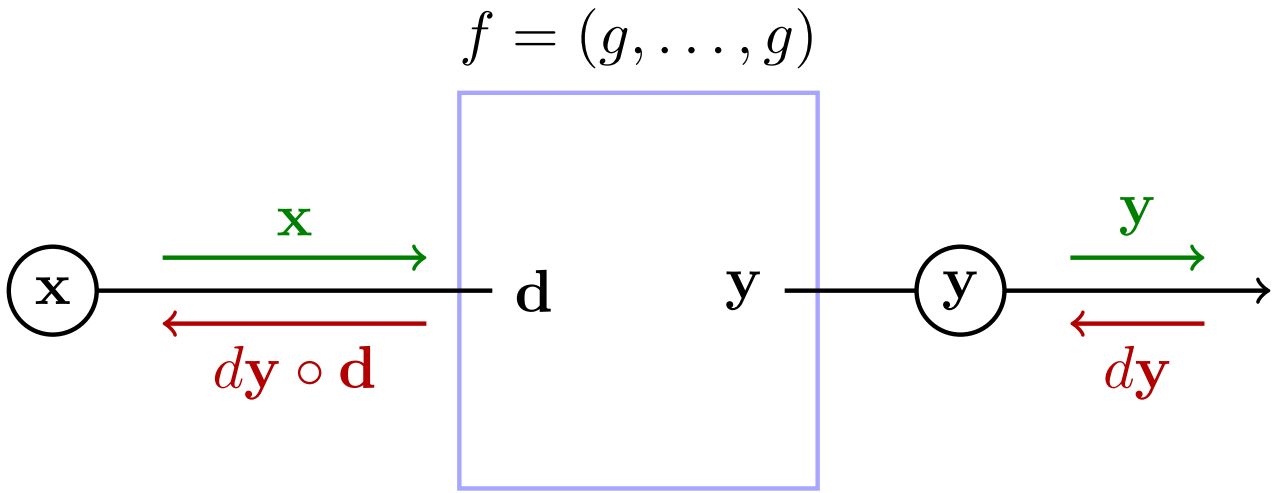

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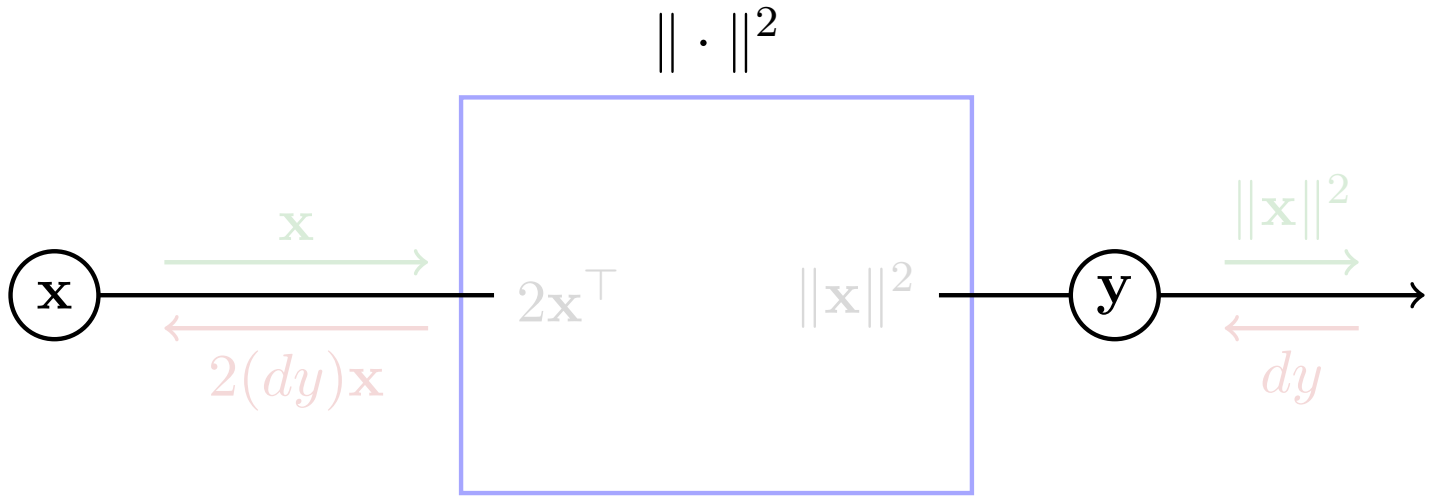
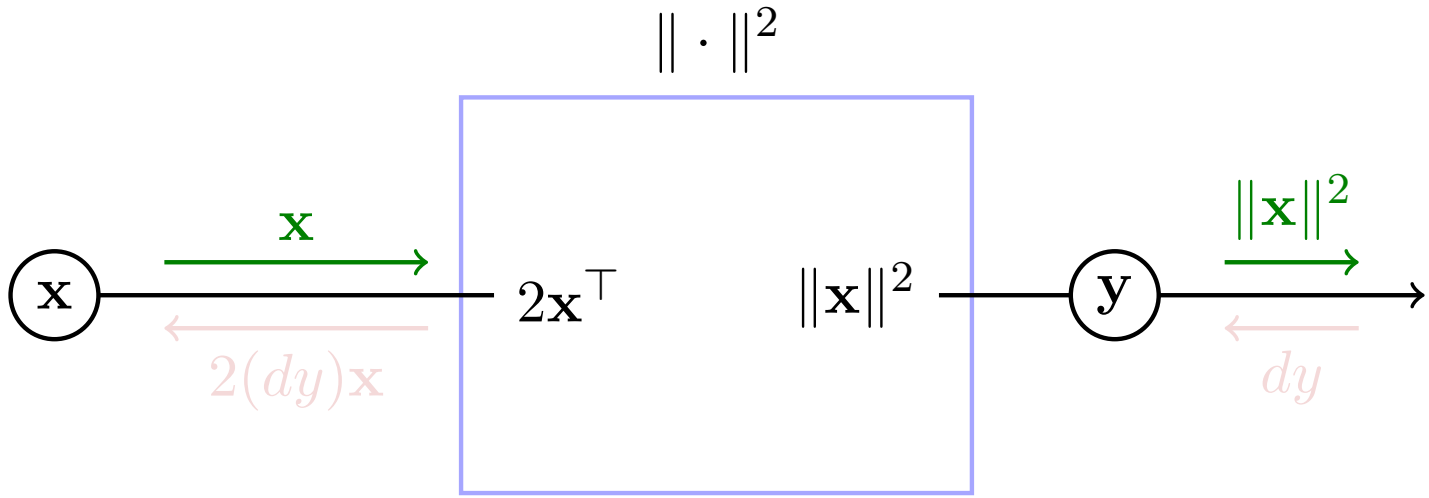
example: squared norm



- if $f(\mathbf{x}) = \|\mathbf{x}\|^2$ then $Df(\mathbf{x}) = 2\mathbf{x}^\top$
- and dy is multiplied by $2\mathbf{x}^\top$; this can be seen by composing a splitter (factor 2) with a dot product (factor $\mathbf{x}^\top$)

example: squared norm



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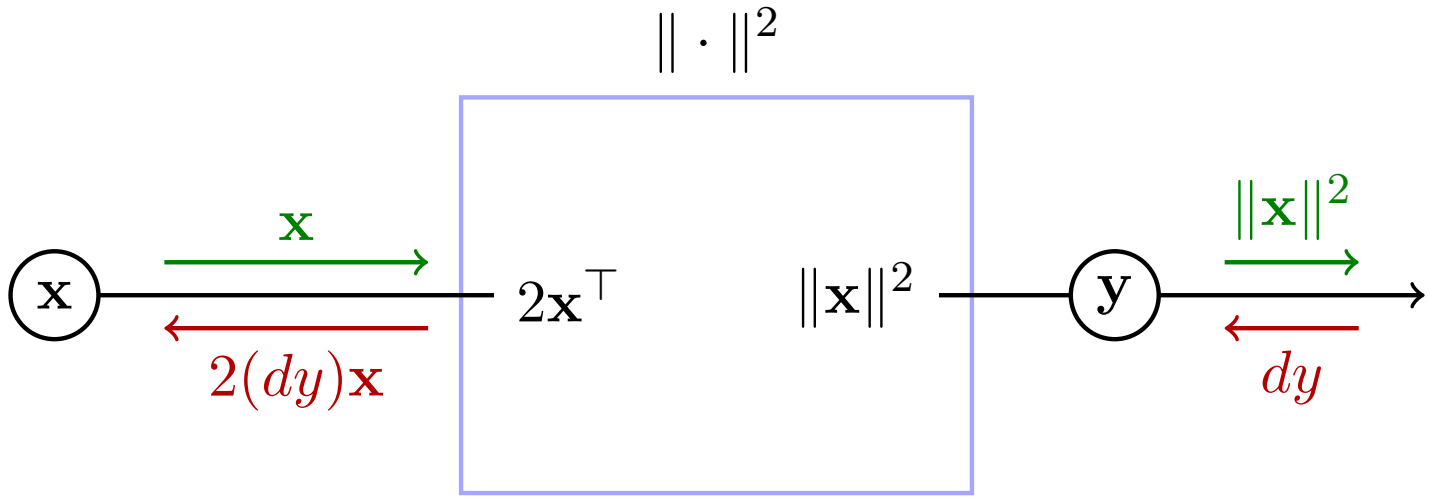
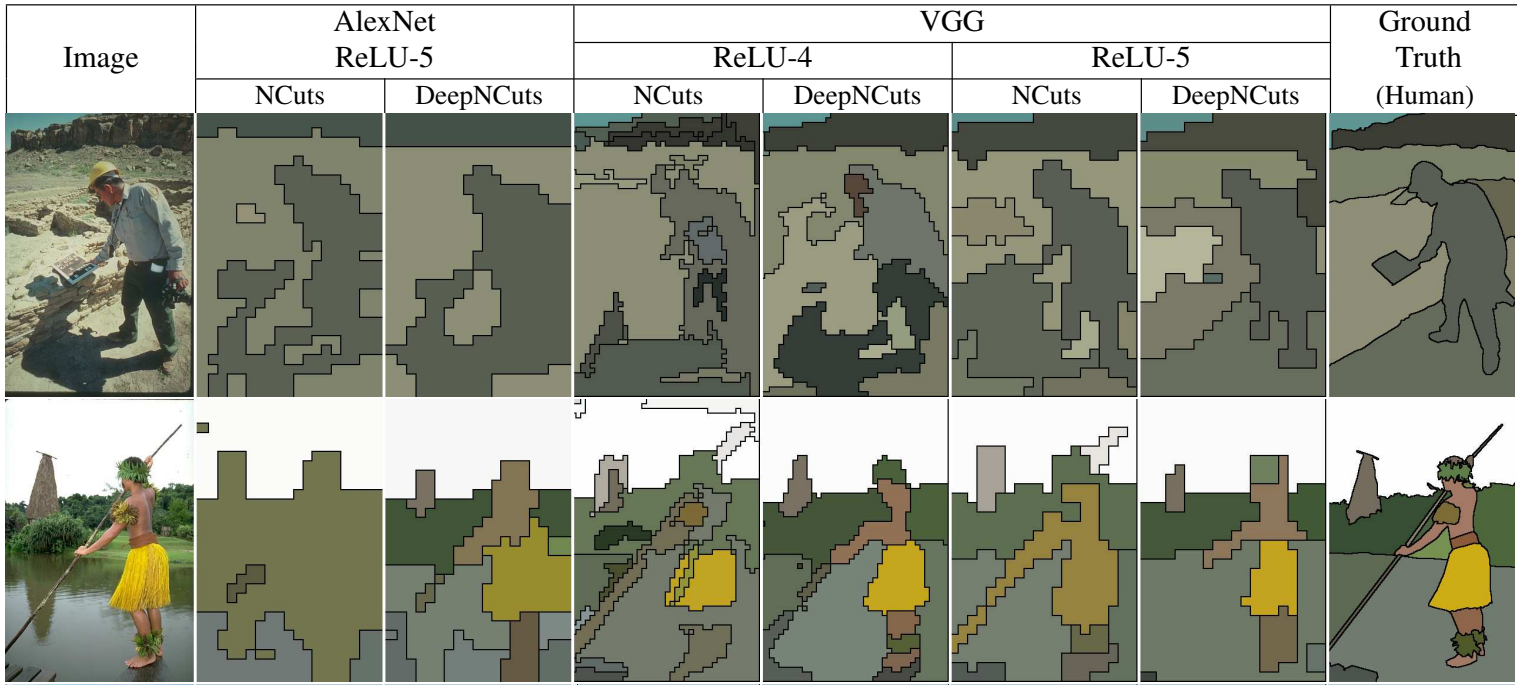
example: squared norm



- if $f(\mathbf{x}) = \|\mathbf{x}\|^2$ then $Df(\mathbf{x}) = 2\mathbf{x}^\top$
- and dy is multiplied by $2\mathbf{x}^\top$; this can be seen by composing a splitter (factor 2) with a dot product (factor $\mathbf{x}^\top$)

matrix derivatives

[Ionescu et al. 2015]



- derivatives for
  - SVD decomposition $A = U\Sigma V^\top$
  - eigenvalue decomposition $A = U\Sigma U^\top$
  - nonlinear matrix functions $f(A) = U\,f(\Sigma)U^\top$
- application to spectral methods for image segmentation

Ionescu Vantzos Sminchisescu. ICCV 2015. Matrix Backpropagation for Deep Networks with Structured Layers.

matrix calculus

- results like these, and many more

$$\frac{\partial A\mathbf{x}}{\partial \mathbf{x}} = A$$
$$\frac{\partial \mathbf{x}^\top A\mathbf{x}}{\partial \mathbf{x}} = \mathbf{x}^\top (A + A^\top)$$
$$\frac{\partial \operatorname{vec}(\mathbf{x}^\top A\mathbf{x})}{\partial \operatorname{vec} A} = \mathbf{x}^\top \otimes \mathbf{x}^\top$$
$$\frac{\partial AXB}{\partial X} = B^\top \otimes A$$
$$\frac{dA^{-1}}{dA} = -(A^{-\top} \otimes A^{-1})$$
$$\frac{d \ln |A|}{dA} = \operatorname{vec}(A^{-\top})^\top$$
$$\frac{\partial \operatorname{tr}(AX)}{\partial X} = \operatorname{vec}(A^\top)^\top$$

Fackler 2005. Notes on Matrix Calculus. `http://www4.ncsu.edu/~pfackler/MatCalc.pdf`

in general

- apparently, we do not need to store the Jacobian matrix $Df(\mathbf{x})$, which may be huge, but only what is needed to compute the partial derivatives in the backward pass
- our function can be decomposed into a directed acyclic graph (DAG) of nodes, called a computational graph
- each time we call the function in the forward pass, a new graph may be constructed if our program contains control flow statements like conditionals and loops; methods supporting this operation are called dynamic

automatic differentiation

[Wengert 1964]

- is the more general set of methods used to automatically evaluate the derivative of a given function at a given input; it is not numerical and not symbolic
- what we call back-propagation here is known as the reverse accumulation mode in this context and makes sense because we compute the gradient of a single scalar quantity with respect to maybe millions of parameters
- forward accumulation makes sense when we need the derivative of many variables with respect to few parameters
- we will use the term automatic differentiation to refer to the process of generating a computer program for the derivatives given the program for the original function

Wengert. CACM 1964. A simple automatic derivative evaluation program.

automatic differentiation: units

automatic differentiation

forward

- evaluation is carried out by units, one calling another
- when invoked, each unit generates a node object
- each node holds the gradient with respect to its unit's inputs, including parameters
- it also holds any information needed for the backward pass

backward

- all gradients are set to zero, except for the gradient with respect to the scalar quantity that is to be optimized (the error), which is set to one
- the $\mathrm{back}()$ method is invoked on the node of this quantity
- this, in turn, triggers the same method on all units that have participated in the forward pass

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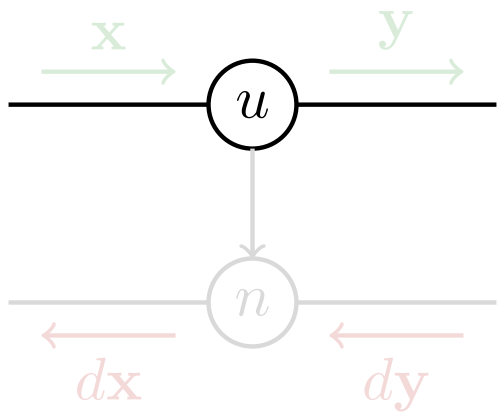
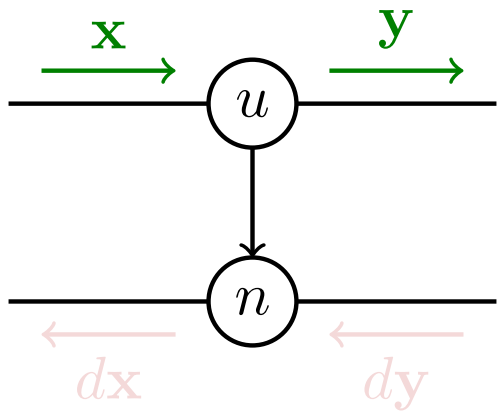
units and nodes



- unit u manually generates node n

units and nodes



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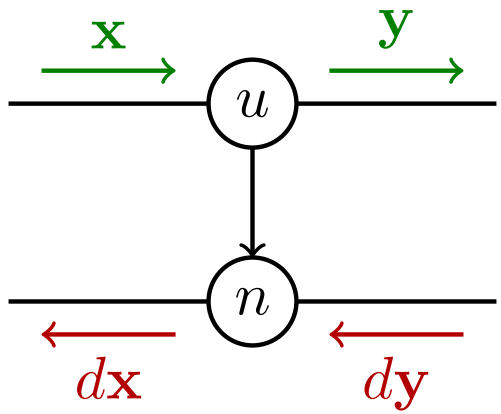

- unit u manually generates node n

units and nodes

- given a function f with derivative Df, a *unit* is a function of the form

$$
\begin{aligned}
&\textbf{def } \text{forward}(\mathbf{x}_1, \ldots, \mathbf{x}_n)\text{:} \\
&\quad \mathbf{y} = f(\mathbf{x}_1, \ldots, \mathbf{x}_n) \\
&\quad \textbf{def } \text{back}(d\mathbf{y}, d\mathbf{x}_1, \ldots, d\mathbf{x}_n)\text{:} \\
&\qquad d\mathbf{x}_1^\top \mathrel{+}= d\mathbf{y}^\top \cdot D_1 f(\mathbf{x}_1, \ldots, \mathbf{x}_n) \\
&\qquad \vdots \\
&\qquad d\mathbf{x}_n^\top \mathrel{+}= d\mathbf{y}^\top \cdot D_n f(\mathbf{x}_1, \ldots, \mathbf{x}_n) \\
&\quad \textbf{return } node(\mathbf{y}, \text{back})
\end{aligned}
$$

- a *node* object:
  - holds $\mathbf{y}$ and an associated derivative $d\mathbf{y}$ of the same shape
  - exposes a method $\text{back}(\mathbf{x}_1, \ldots, \mathbf{x}_n)$ where $\mathbf{x}_i$ can be *nodes*
  - automatically adds its own $d\mathbf{y}$ as first argument
  - if an input $\mathbf{x}_i$ is a *node*, extracts the derivative part $d\mathbf{x}_i$
  - otherwise, $d\mathbf{x}_i$ is an object for which operation $+=$ is ignored

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the affine unit

- input vectors are represented as rows of $m \times p$ input matrix X where m is the mini-batch size and p the input dimension
- parameters are represented by $p \times q$ weight matrix W and $1 \times q$ bias vector $\mathbf{b}$ where q is the output dimension
- the unit is defined as

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&\textbf{def } \mathrm{affine}(X, (W, \mathbf{b})): \\
&\quad A = \mathrm{dot}(X, W) + \mathbf{b} \\
&\quad \textbf{def } \mathrm{back}(dA, dX, (dW, d\mathbf{b})): \\
&\quad\quad dW \mathrel{+}= \mathrm{dot}(X^\top, dA) \\
&\quad\quad d\mathbf{b} \mathrel{+}= \mathrm{sum}_0(dA) \\
&\quad\quad dX \mathrel{+}= \mathrm{dot}(dA, W^\top) \\
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the affine unit in math

forward

- input $X \in \mathbb{R}^{m \times p}$, $W \in \mathbb{R}^{p \times q}$, $\mathbf{b} \in \mathbb{R}^q$, output $A \in \mathbb{R}^{m \times q}$

$$A = f(X; W, \mathbf{b}) := XW + \mathbf{1}_m \mathbf{b}^\top$$

observe that in the code, addition of $\mathbf{b}$ is handled by broadcasting

backward

- if $\mathbf{a}_i$, $\mathbf{w}_i$ is the i-th column of A, W, it is known that

$$\frac{\partial \mathbf{a}_i}{\partial \mathbf{w}_i} = \frac{\partial (X\mathbf{w}_i)}{\partial \mathbf{w}_i} = X$$

and there are no other dependencies, so by the chain rule

$$d\mathbf{w}_i^\top := \frac{\partial}{\partial \mathbf{w}_i} = \frac{\partial}{\partial \mathbf{a}_i} \cdot \frac{\partial \mathbf{a}_i}{\partial \mathbf{w}_i} = d\mathbf{a}_i^\top \cdot X$$

- finally, the partial derivative with respect to W

$$dW = (dA^\top X)^\top = X^\top dA$$

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the affine unit in math

- by symmetry, writing $A^\top = W^\top X^\top + \mathbf{b}\mathbf{1}_m^\top$ and using the previous result for dW, we find $dX^\top = (W^\top)^\top dA^\top$ or

$$dX = (dA)W^\top$$

- again, by replacing X and W by $\mathbf{1}_m$ and $\mathbf{b}^\top$ respectively in the previous result for dW,

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- observe that distributing $\mathbf{b}$ in the forward yields a sum in the backward

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the logistic unit

- the input is an $m \times q$ activation matrix A and the $m \times k$ one-of-k encoded target matrix, where k is the number of classes
- there are no parameters
- the unit integrates softmax with average cross-entropy loss

$$
\begin{aligned}
&\textbf{def } \mathrm{logistic}(A, T)\text{:} \\
&\quad E = \exp(A) \\
&\quad Y = E / \mathrm{sum}_1(E) \\
&\quad C = -\mathrm{sum}_1(T * \log(Y)) \\
&\quad D = \mathrm{sum}_0(C)/m \\
&\quad \textbf{def } \mathrm{back}(dD, dA, \_)\text{:} \\
&\quad\quad dA \mathrel{+}= dD * (Y - T)/m \\
&\quad \textbf{return } node(D, \mathrm{back})
\end{aligned}
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  return $node(D, \mathrm{back})$

the logistic unit in math

forward

- E is given element-wise as $e_{ij} = \exp(a_{ij})$, and $m \times q$ matrix Y is row-normalized as

$$Y = (\mathrm{diag}(E\mathbf{1}_k))^{-1}E$$

- the i-th row of Y is the $\mathrm{softmax}$ output of the i-th input sample representing the k posterior class probabilities
- C is actually a $m \times 1$ column vector and its i-th element represents the cross-entropy loss of the i-th input sample

$$c_i = -\sum_{j=1}^{k} t_{ij} \log(y_{ij})$$

- finally, $D = \frac{1}{m}\sum_{i=1}^{m} c_i$ is a scalar and represents the average cross-entropy (data) error over the mini-batch

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the logistic unit in math

backward

- if $\mathbf{a}_i^\top$, $\mathbf{y}_i^\top$, $\mathbf{t}_i^\top$ is the i-th row of A, Y, T, the derivative of the cross-entropy loss is, according to what we have seen,

$$\frac{\partial c_i}{\partial \mathbf{a}_i}(\mathbf{a}_i, \mathbf{t}_i) = (\boldsymbol{\sigma}(\mathbf{a}_i) - \mathbf{t}_i)^\top = (\mathbf{y}_i - \mathbf{t}_i)^\top$$

- since D is the average of the individual sample losses c_i, the derivative of the total error, which is 1 by default, is distributed over the samples with a factor of $\frac{1}{m}$

$$dA^\top = \frac{1}{m}(Y - T) \cdot dD$$

why integrate $\mathrm{softmax}$ with cross-entropy?

- the simplified formula is faster compared to blind application of back-propagation at the level of elementary functions
- if this is not convincing, try evaluating the binary cross-entropy loss

$$\ell(x) := \ln(1 + e^{-x})$$

- $\ell(-1) = 1.3133$
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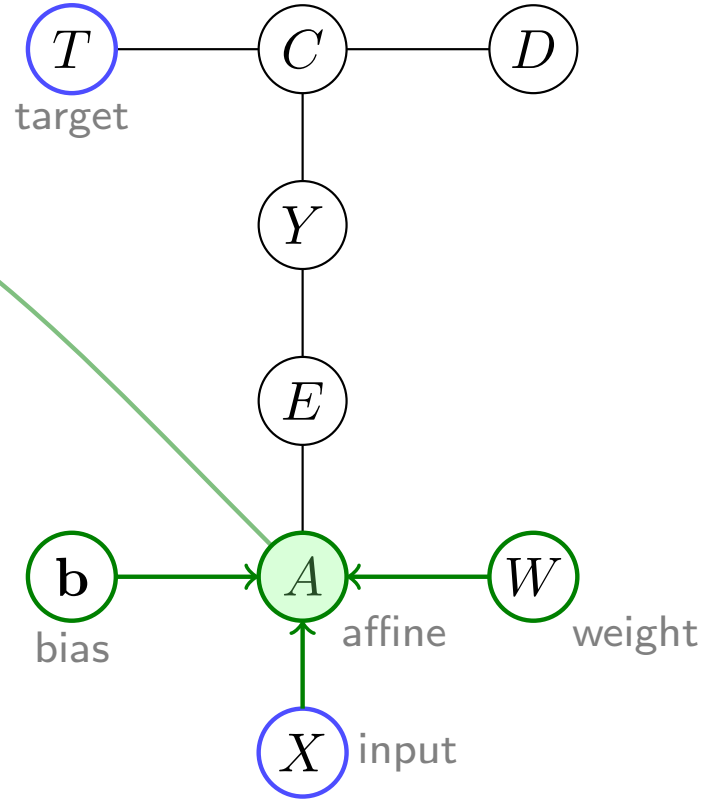
back-propagation

forward

$$A = \mathrm{dot}(Z, W) + \mathbf{b}$$



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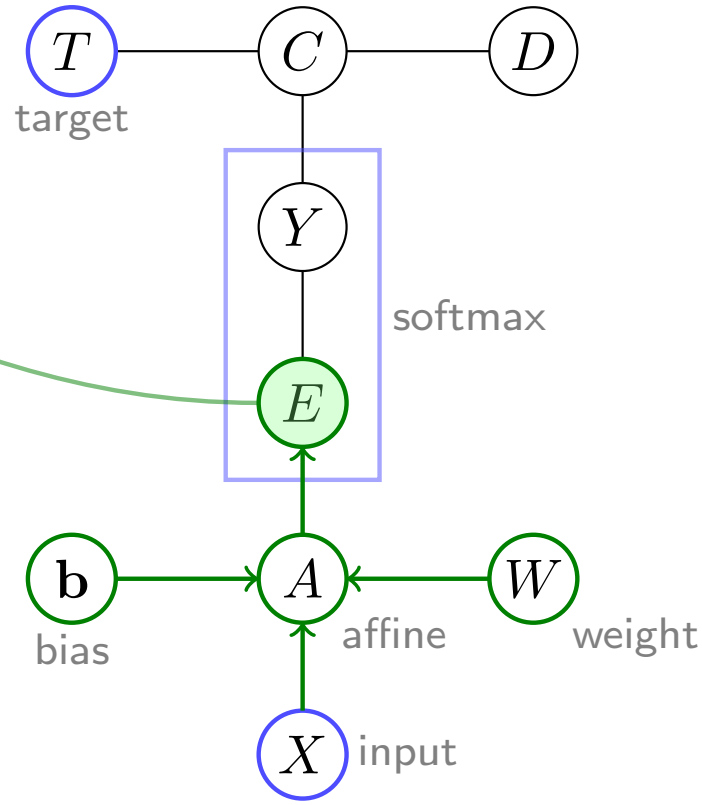

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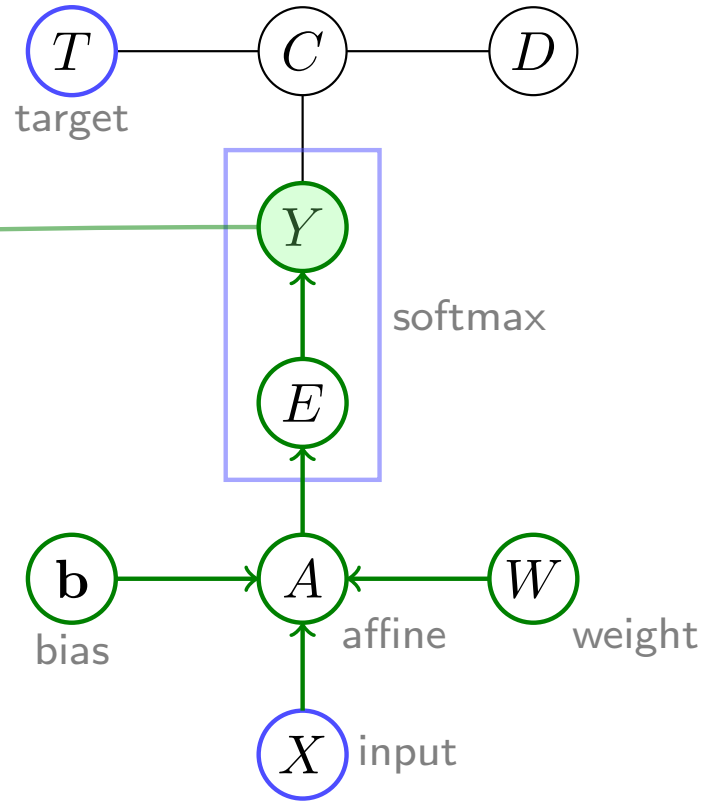

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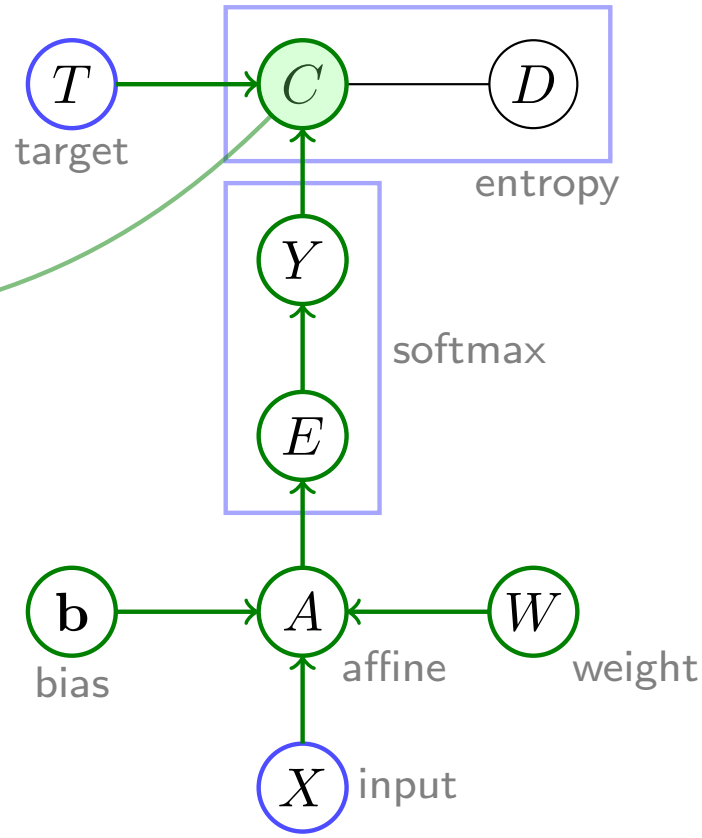

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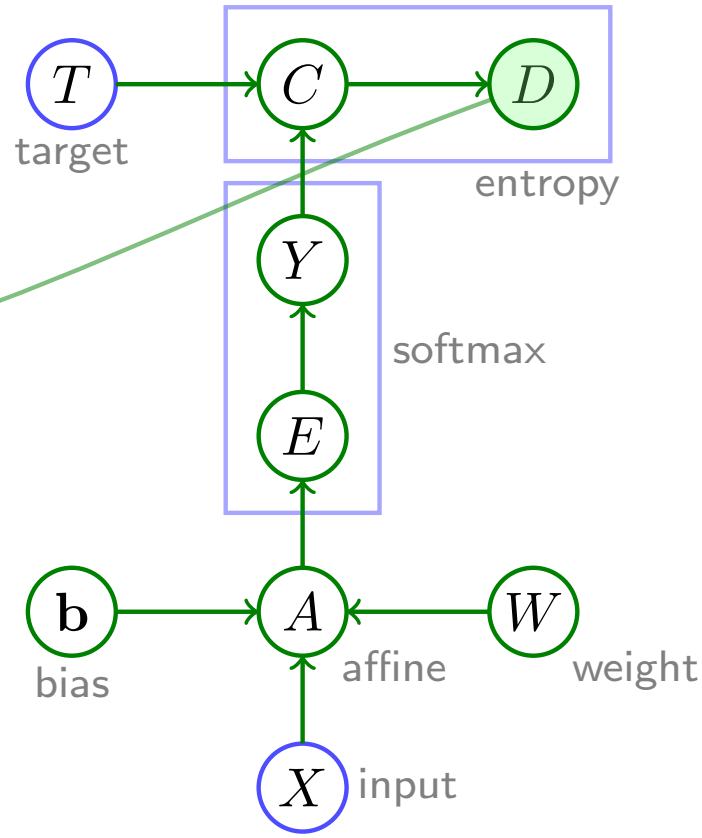

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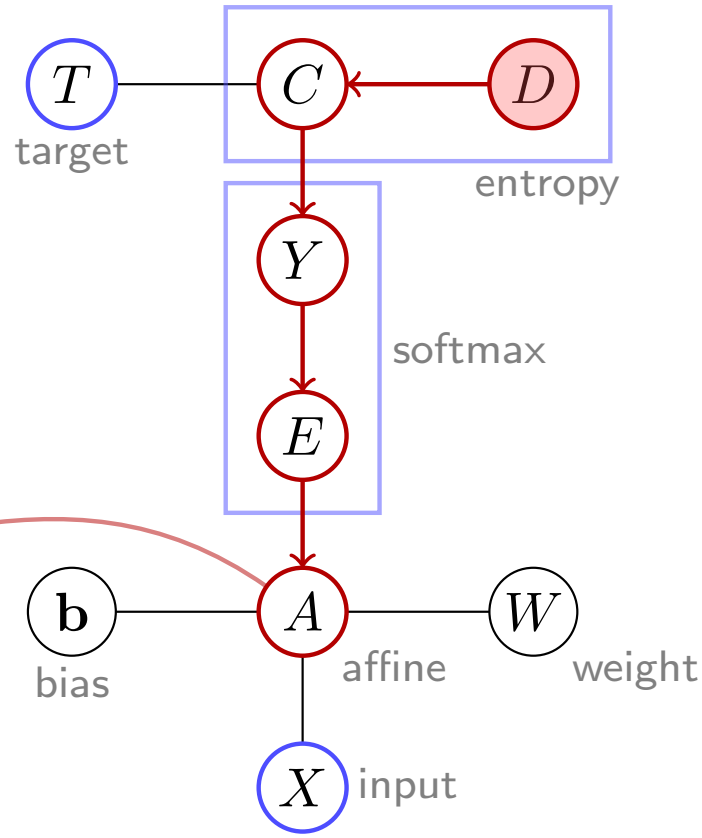

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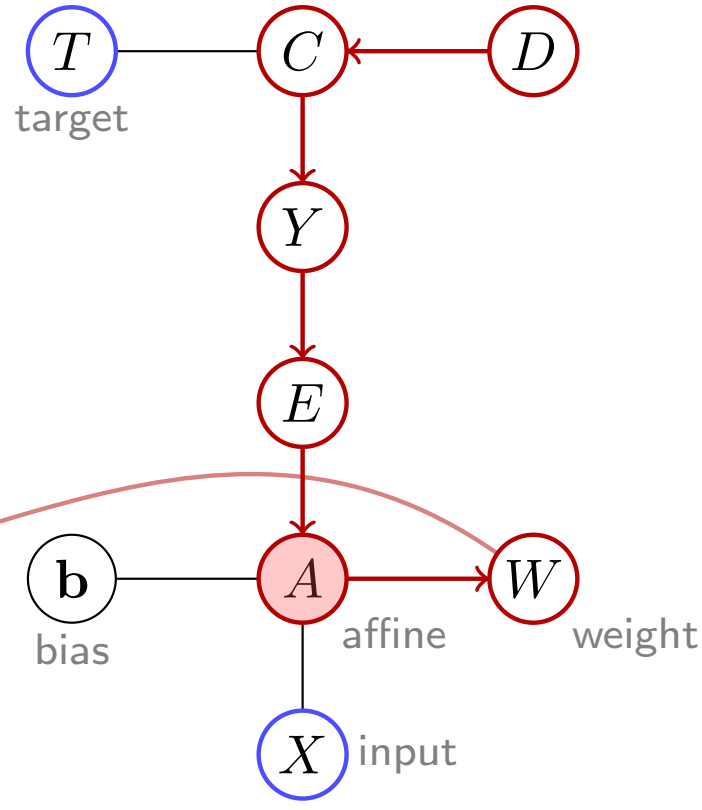
$$dW \mathrel{+}= \mathrm{dot}(Z^\top, dA)$$
$$d\mathbf{b} = \mathrm{sum}_0(dA)$$



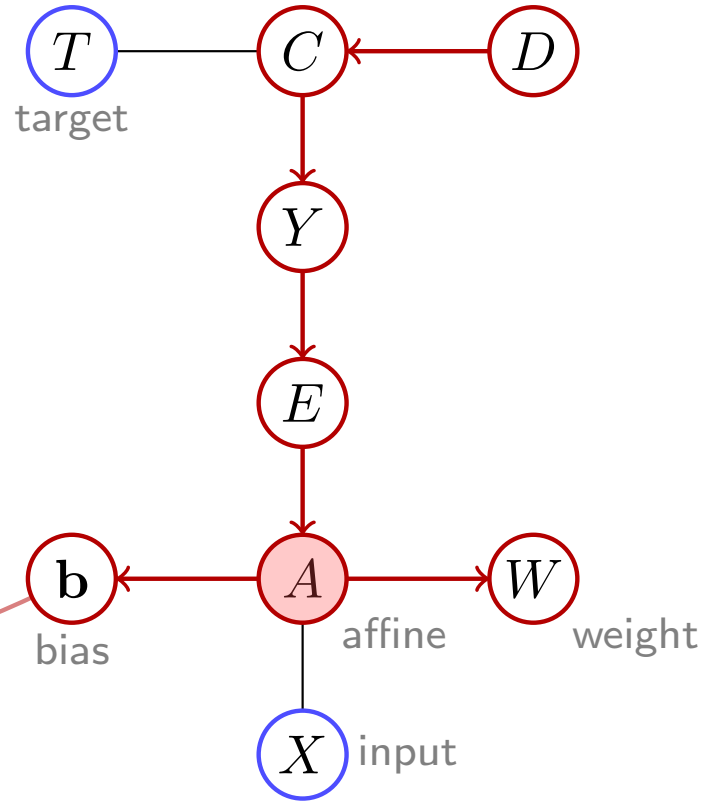
back-propagation

forward

$$A = \mathrm{dot}(Z, W) + \mathbf{b}$$
$$E = \exp(A)$$
$$Y = E / \mathrm{sum}_1(E)$$
$$C = -\mathrm{sum}_1(T * \log(Y))$$
$$D = \mathrm{sum}_0(C)/m$$

backward

$$dA = dD * (Y - T)/m$$
$$dW \mathrel{+}= \mathrm{dot}(Z^\top, dA)$$
$$d\mathbf{b} = \mathrm{sum}_0(dA)$$



automatic differentiation

forward

$$
\begin{aligned}
A &= \mathrm{dot}(Z, W) + \mathbf{b} \\
E &= \exp(A) \\
Y &= E / \mathrm{sum}_1(E) \\
C &= -\mathrm{sum}_1(T * \log(Y)) \\
D &= \mathrm{sum}_0(C)/m
\end{aligned}
$$

backward

$$
\begin{aligned}
dA &= dD * (Y - T)/m \\
dW &+= \mathrm{dot}(Z^\top, dA) \\
d\mathbf{b} &= \mathrm{sum}_0(dA)
\end{aligned}
$$

now we organize forward and backward code into units

automatic differentiation

forward

$A = \mathrm{dot}(Z, W) + \mathbf{b}$
$E = \exp(A)$
$Y = E / \mathrm{sum}_1(E)$
$C = -\mathrm{sum}_1(T * \log(Y))$
$D = \mathrm{sum}_0(C)/m$

backward

$dA = dD * (Y - T)/m$
$dW \mathrel{+}= \mathrm{dot}(Z^\top, dA)$
$d\mathbf{b} = \mathrm{sum}_0(dA)$

def affine$(X, (W, \mathbf{b}))$:
  $A = \mathrm{dot}(X, W) + \mathbf{b}$
  def back$(dA, dX, (dW, d\mathbf{b}))$:
    $dW \mathrel{+}= \mathrm{dot}(X^\top, dA)$
    $d\mathbf{b} \mathrel{+}= \mathrm{sum}_0(dA)$
    $dX \mathrel{+}= \mathrm{dot}(dA, W^\top)$
  return $node(A, \mathrm{back})$

automatic differentiation

forward

$A = \text{affine}(Z, (W, \mathbf{b}))$
$E = \exp(A)$
$Y = E / \text{sum}_1(E)$
$C = -\text{sum}_1(T * \log(Y))$
$D = \text{sum}_0(C)/m$

backward

$dA = dD * (Y - T)/m$
$A.\,\text{back}(Z, (W, \mathbf{b}))$

def $\text{affine}(X, (W, \mathbf{b}))$:
  $A = \text{dot}(X, W) + \mathbf{b}$
  def $\text{back}(dA, dX, (dW, d\mathbf{b}))$:
    $dW \mathrel{+}= \text{dot}(X^\top, dA)$
    $d\mathbf{b} \mathrel{+}= \text{sum}_0(dA)$
    $dX \mathrel{+}= \text{dot}(dA, W^\top)$
  return $node(A, \text{back})$

automatic differentiation

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$A = \text{affine}(Z, (W, \mathbf{b}))$

$E = \exp(A)$
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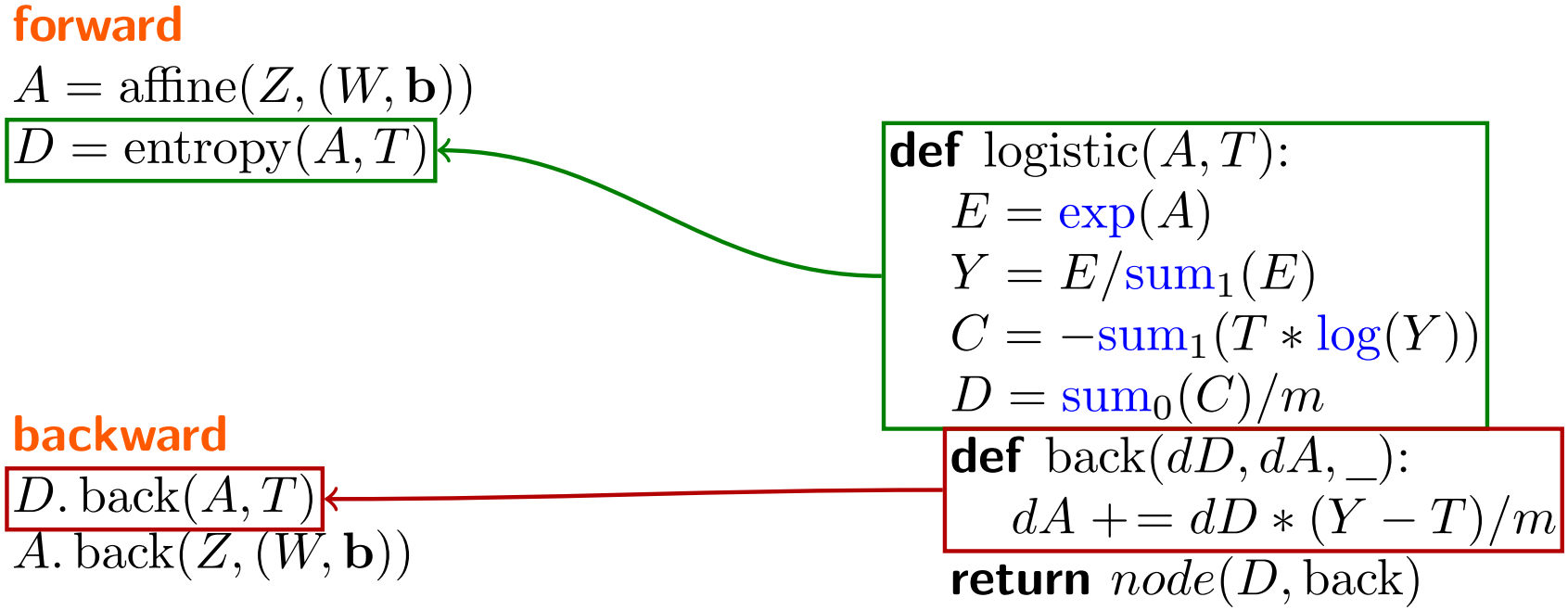
$C = -\text{sum}_1(T * \log(Y))$
$D = \text{sum}_0(C)/m$

backward

$dA = dD * (Y - T)/m$
$A.\text{back}(Z, (W, \mathbf{b}))$

def $\text{logistic}(A, T)$:
  $E = \exp(A)$
  $Y = E/\text{sum}_1(E)$
  $C = -\text{sum}_1(T * \log(Y))$
  $D = \text{sum}_0(C)/m$
  def $\text{back}(dD, dA, \_)$:
    $dA \mathrel{+}= dD * (Y - T)/m$
  return $node(D, \text{back})$

automatic differentiation



automatic differentiation: functions

the relu unit

- relu is an element-wise activation function; its input is activation matrix A and returns matrix Z of the same size
- its backward pass behaves like a switch

```
def relu(A):
    Z = max(0, A)
    def back(dZ, dA):
        dA += dZ * (Z > 0)
    return node(Z, back)
```

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    $dA \mathrel{+}= dZ * (Z > 0)$
  return $node(Z, \mathrm{back})$

the decay unit

- it takes as input a tuple or list of weight matrices W of any size and returns the weight decay error term $\frac{\lambda}{2}\|w\|^2$ for each $w \in W$, where $\|\cdot\|_F$ is the Frobenius norm
- the backward derivative is proportional to w, as for the ℓ_2 norm

```
def decay(W):
    R = λ/2 * sum(||w||_F^2 for w in W)
    def back(dR, dW):
        for (w, dw) in zip(W, dW):
            dw += dR * λ * w
    return node(R, back)
```

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def $\mathrm{decay}(W)$:
  $R = \frac{\lambda}{2} * \mathrm{sum}(\|w\|_F^2$ **for** w **in** $W)$
  def $\mathrm{back}(dR, dW)$:
    for (w, dw) **in** $\mathrm{zip}(W, dW)$:
      $dw \mathrel{+}= dR * \lambda * w$
  return $node(R, \mathrm{back})$

the add unit

- it takes as input a tuple or list of matrices (or vectors, or scalars) X of the same size and returns their sum
- its backward pass distributes the derivative to all input branches

$$
\begin{array}{l}
\textbf{def } \mathrm{add}(X): \\
\quad S = \mathrm{sum}(X) \\
\quad \textbf{def } \mathrm{back}(dS, dX): \\
\quad\quad \textbf{for } dx \textbf{ in } dX: \\
\quad\quad\quad dx \mathrel{+}= dS \\
\quad \textbf{return } node(S, \mathrm{back})
\end{array}
$$

- operator $+$ is overloaded for $nodes$ such that $A + B$ means $\mathrm{add}((A, B))$

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- operator $+$ is overloaded for $node$s such that $A + B$ means $\mathrm{add}((A, B))$

the loss function

- it takes as input the activation matrix A, the target matrix T and the weight matrix list W
- it calls the logistic unit on (A, T) and the decay unit on W, and returns the sum of the two scalar terms

def loss(A, T, W):
  $L = \text{logistic}(A, T) + \text{decay}(W)$
  return $block(L)$

- addition is handled by add and the error derivative flows backward to both branches

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  return $block(L)$

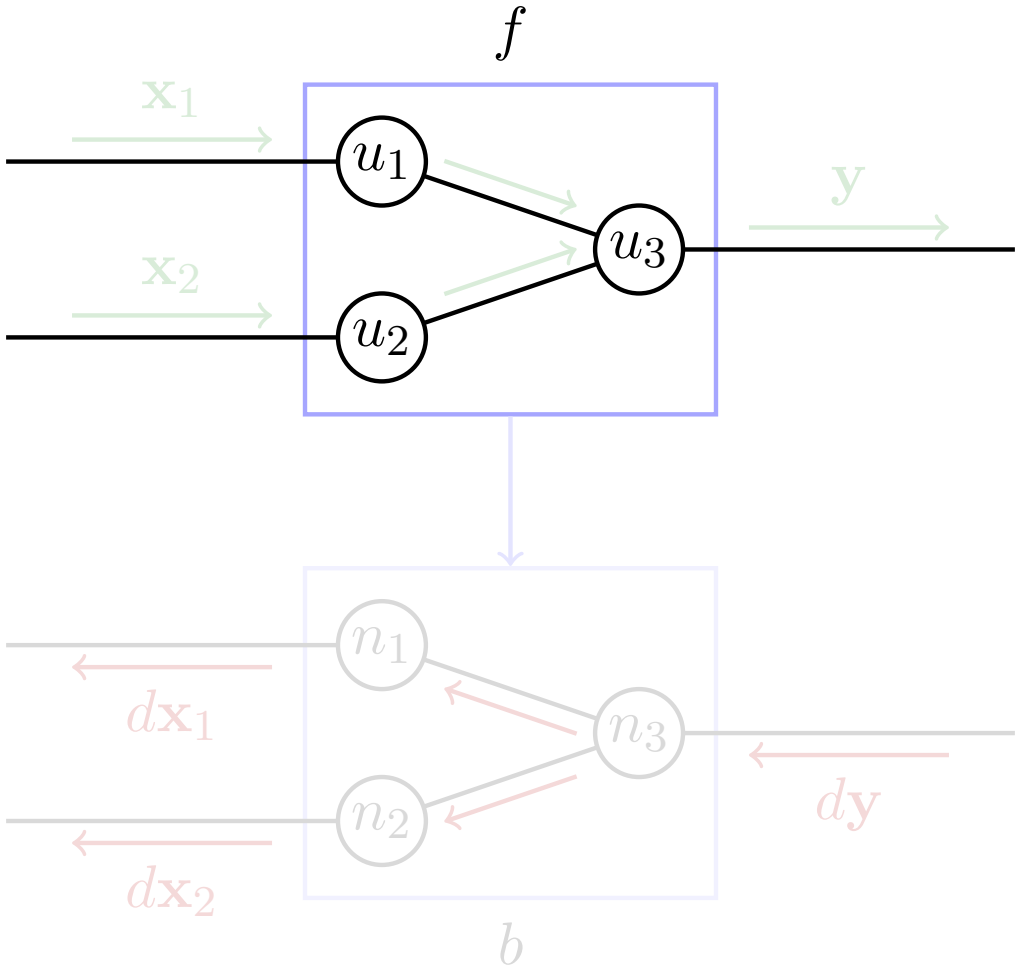
- addition is handled by add and the error derivative flows backward to both branches

the model function

- this is a two-layer network model where an affine layer is followed by a relu activation function and another affine layer
- the parameter tuple $U_i = (W_i, \mathbf{b}_i)$ for layer i contains a weight matrix W_i and a bias vector $\mathbf{b}_i$
- unit calls are nested like every other function

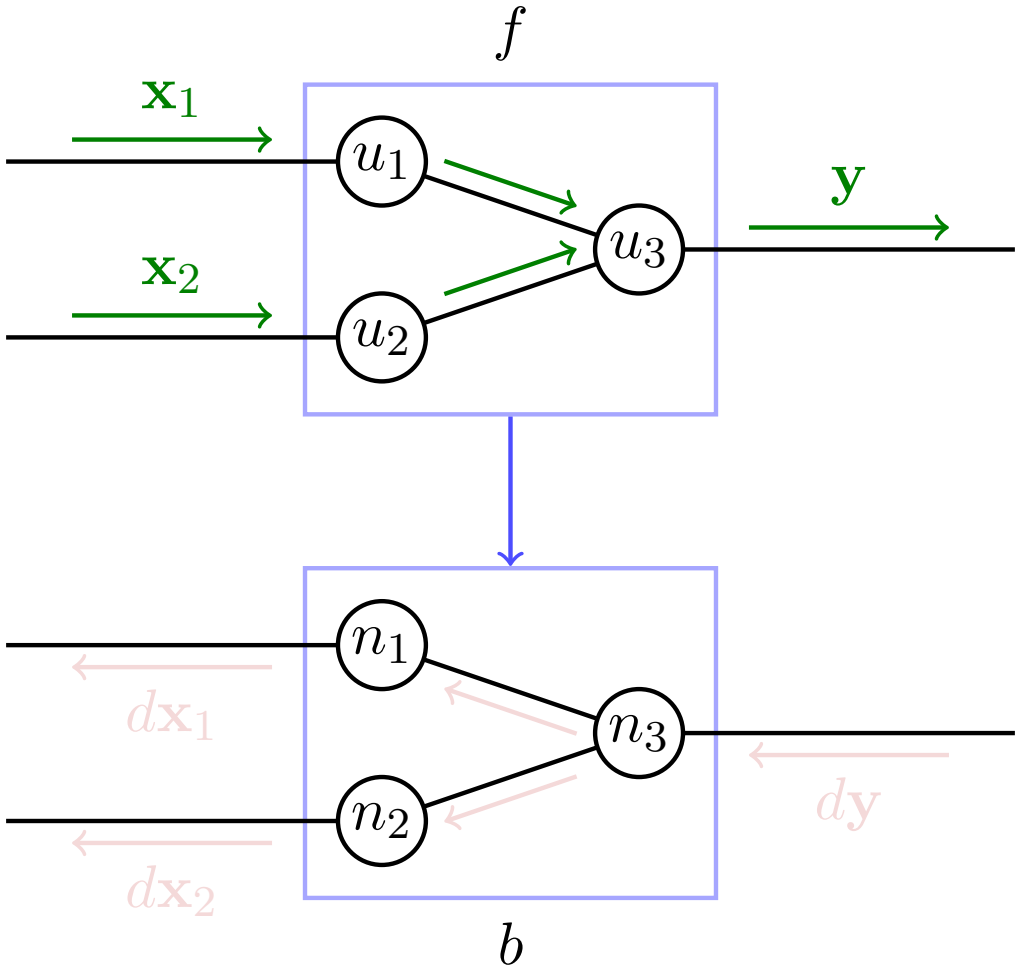
$$
\begin{aligned}
&\textbf{def } \mathrm{model}(X, (U_1, U_2)):\\
&\quad A = \mathrm{affine}(\mathrm{relu}(\mathrm{affine}(X, U_1)), U_2)\\
&\quad \textbf{return } block(A)
\end{aligned}
$$

functions and blocks



- function f containing units u_1, u_2, u_3
- f dynamically generates block b containing nodes n_1, n_2, n_3, manually generated by u_1, u_2, u_3 respectively

functions and blocks



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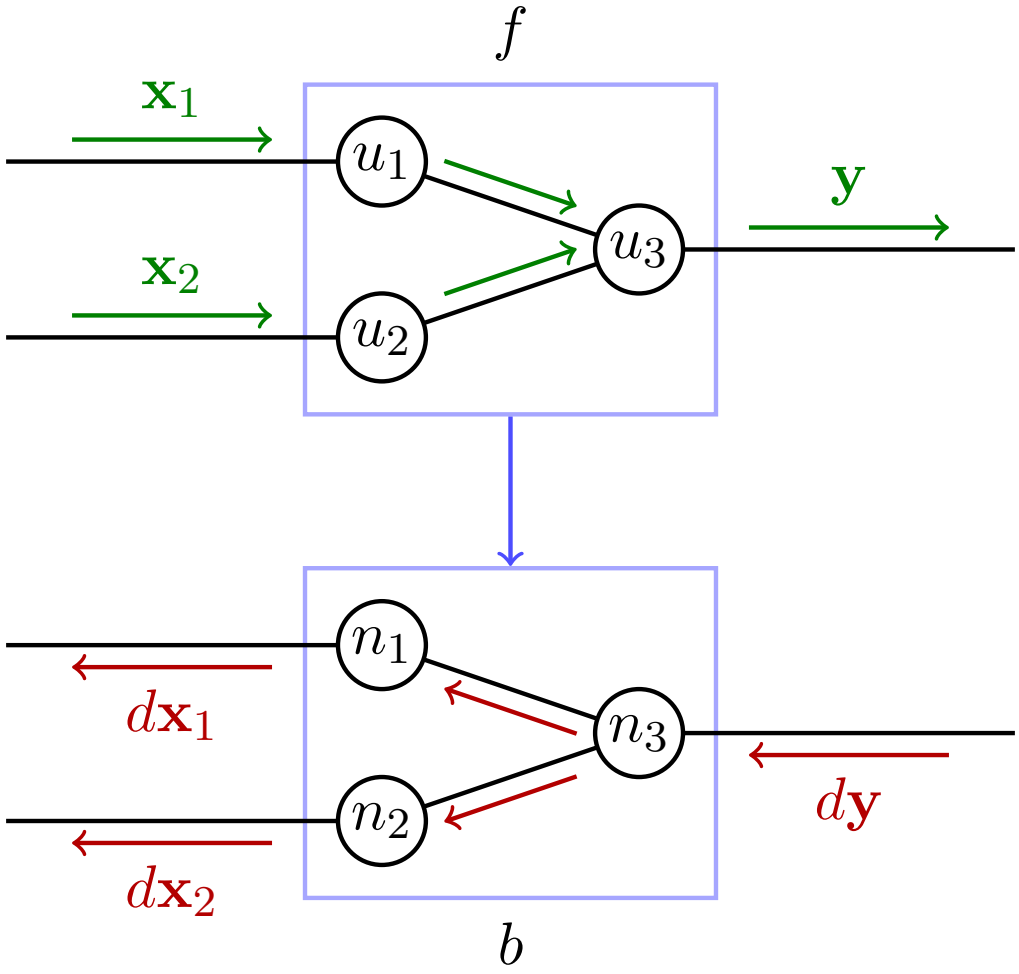

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functions and blocks

- a *function* is a function of the following form, where code is arbitrary but computation takes place through calls to *units* or *functions*

$$
\begin{aligned}
&\textbf{def } name(\mathbf{x}_1, \ldots, \mathbf{x}_n)\text{:} \\
&\quad \langle \text{code generating the following} \rangle \\
&\quad \mathbf{r}_1 = \mathrm{call}_1(\mathbf{a}_1, \ldots, \mathbf{a}_{n_1}) \\
&\quad \vdots \\
&\quad \mathbf{r}_s = \mathrm{call}_s(\mathbf{a}_1, \ldots, \mathbf{a}_{n_s}) \\
&\quad \textbf{return } block(\mathbf{r}_s)
\end{aligned}
$$

- all calls are recorded as a list of *units* or *functions* by call order, each associated with a list of arguments
- a *block* object is a *node*, but
  - its method $\mathrm{back}()$ does not add its own derivative in the arguments
  - its method $\mathrm{back}()$ is automatically generated and its body calls the recorded functions with the same arguments in reverse order

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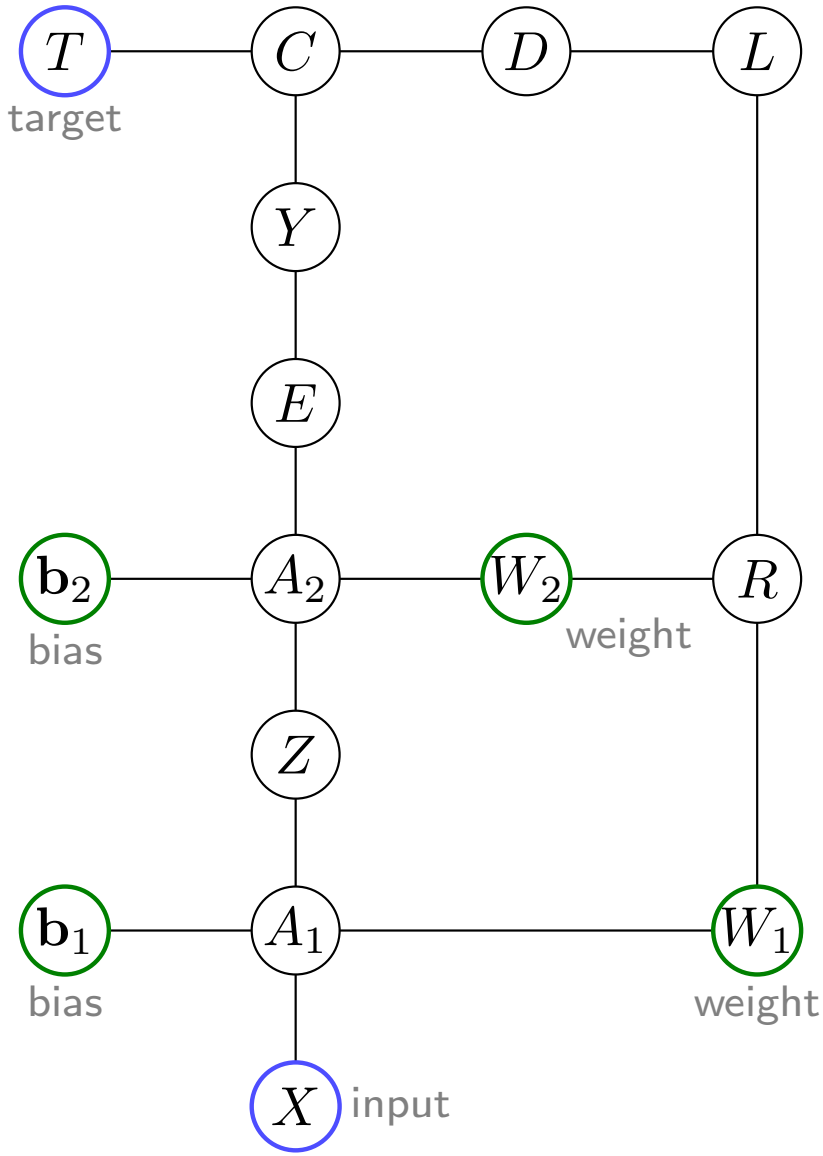
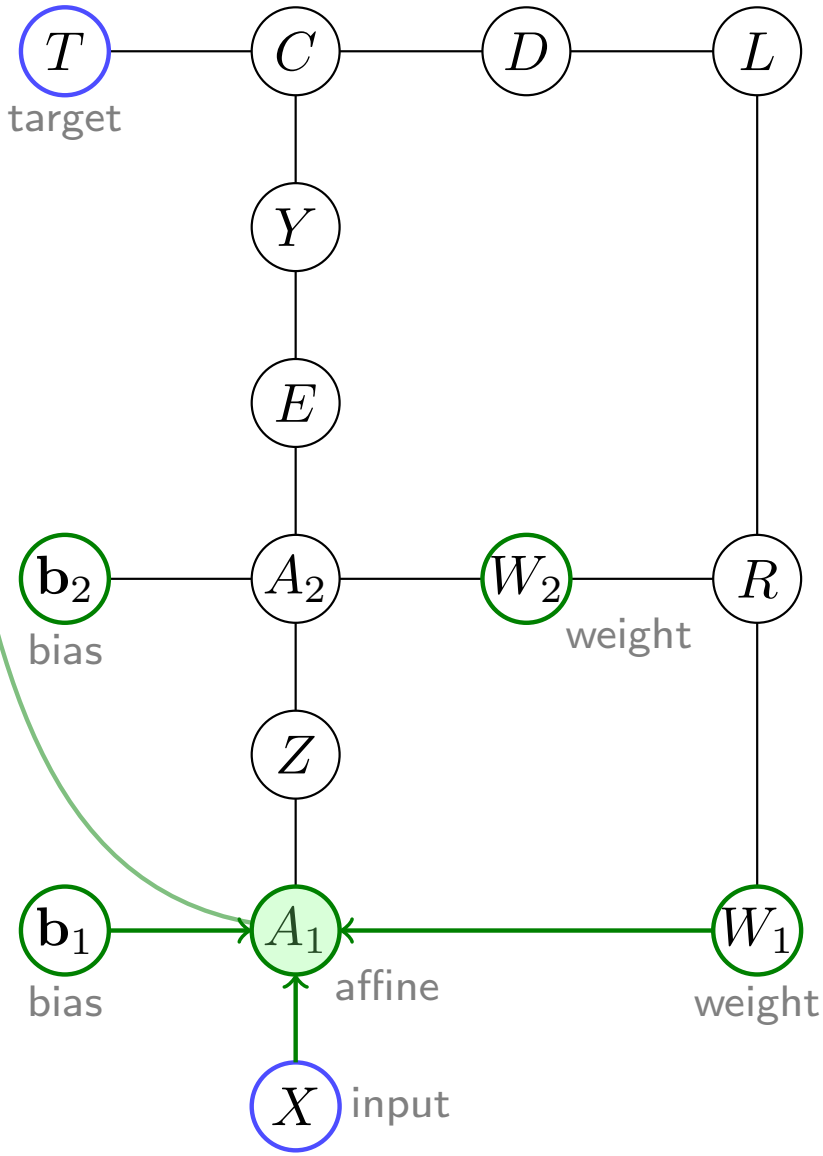
back-propagation



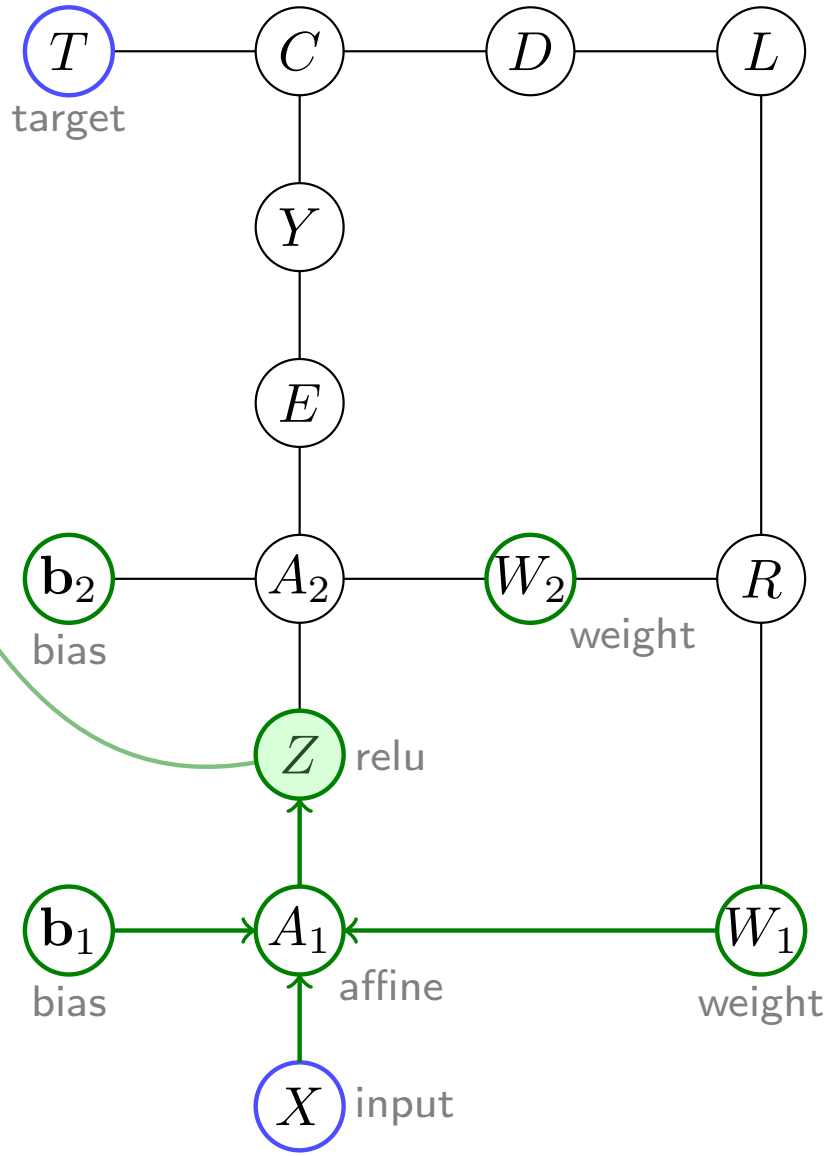
back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$



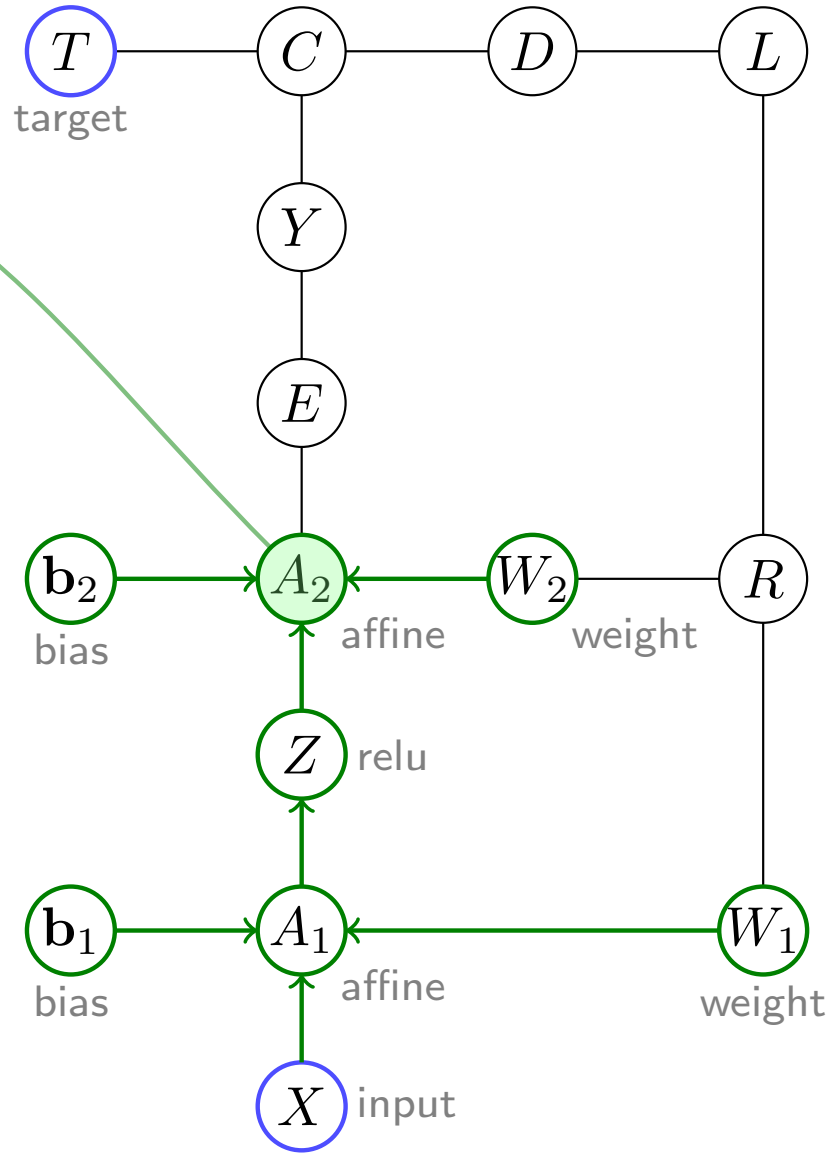
back-propagation

$$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$$
$$Z = \max(0, A_1)$$



back-propagation

$$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$$
$$Z = \max(0, A_1)$$
$$\boxed{A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2}$$



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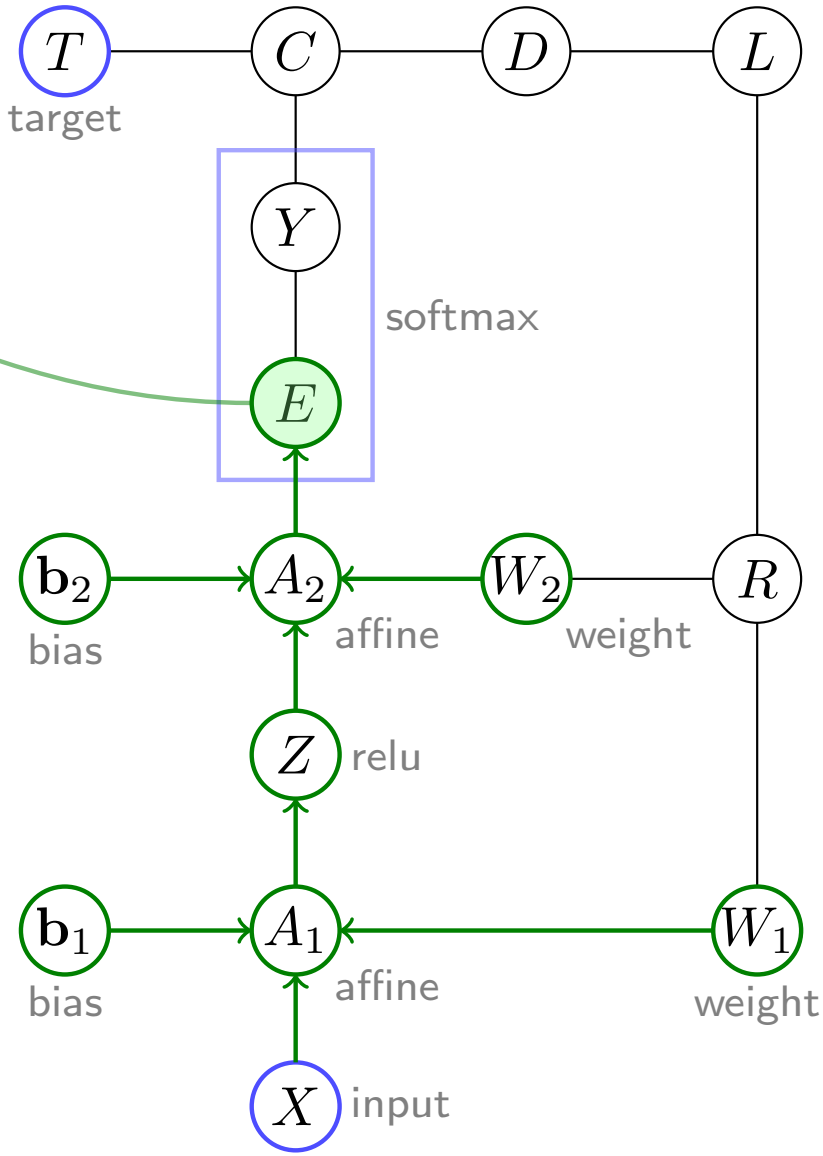
$$Y = E / \text{sum}_1(E)$$
$$C = -\text{sum}_1(T * \log(Y))$$
$$D = \text{sum}_0(C)/m$$



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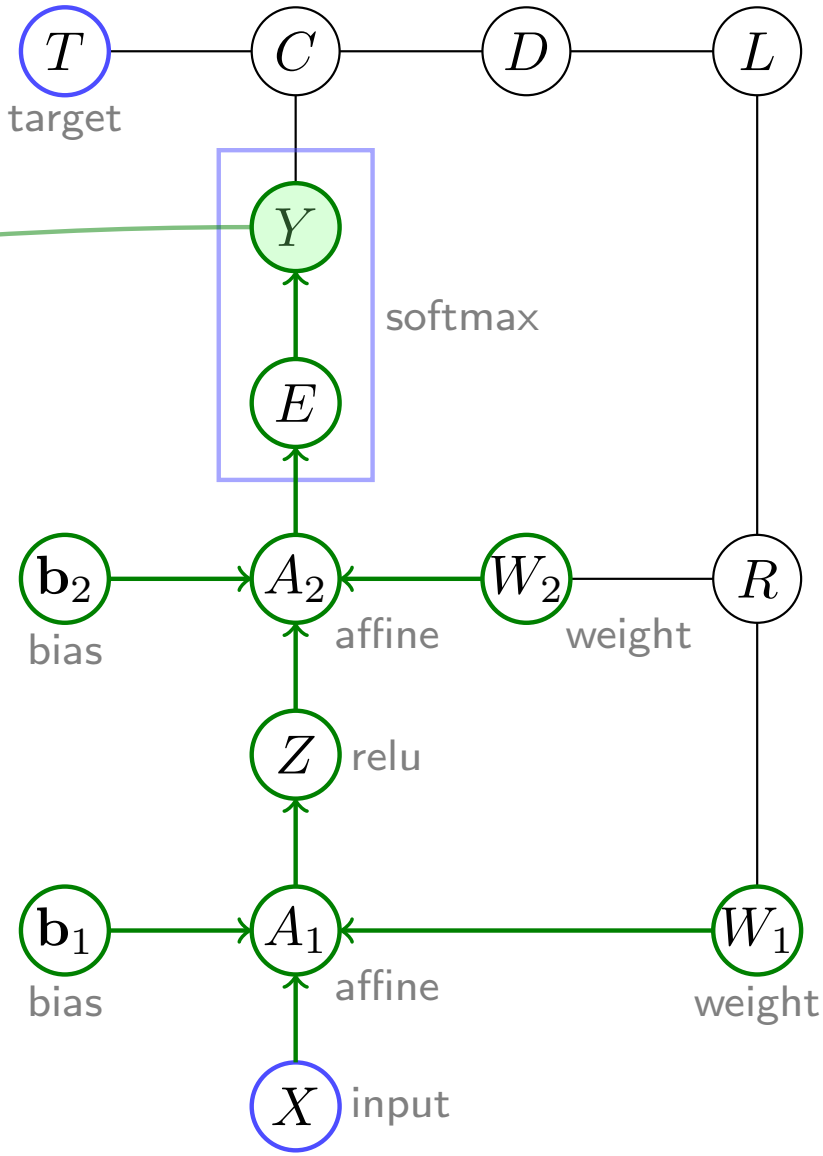

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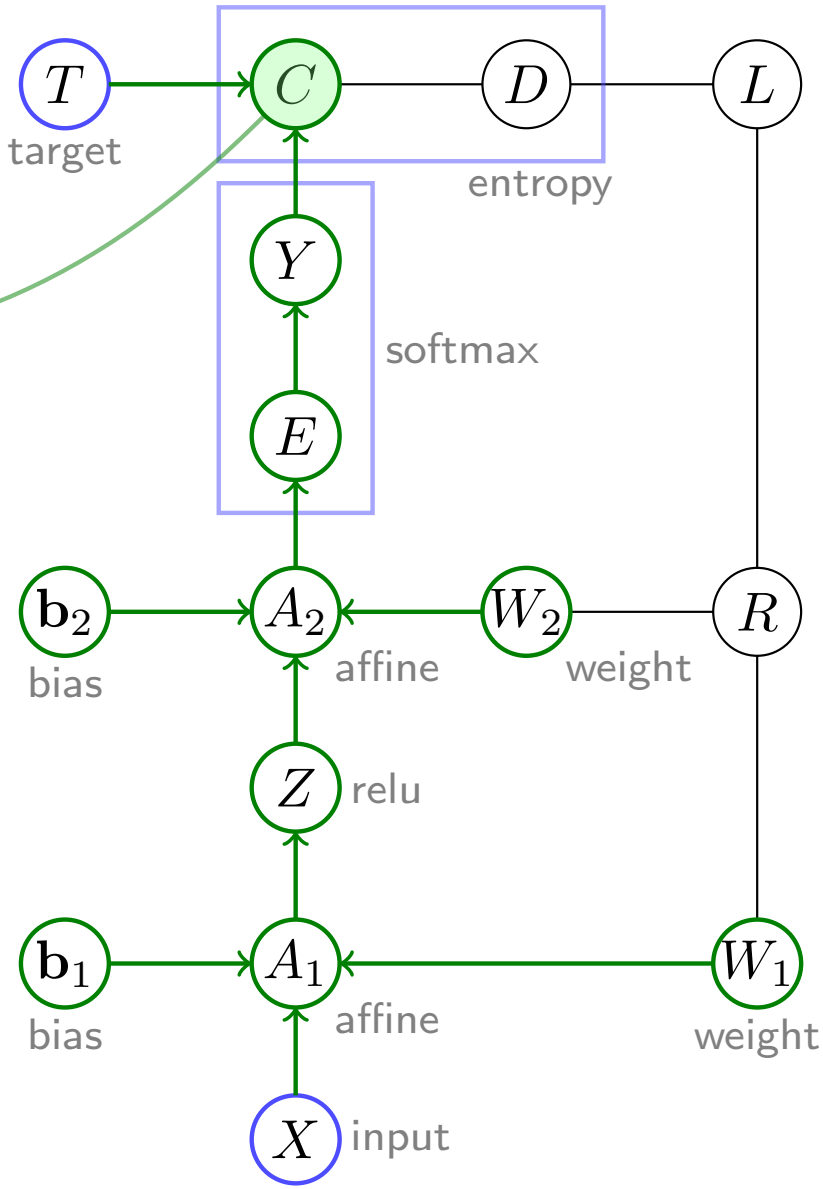

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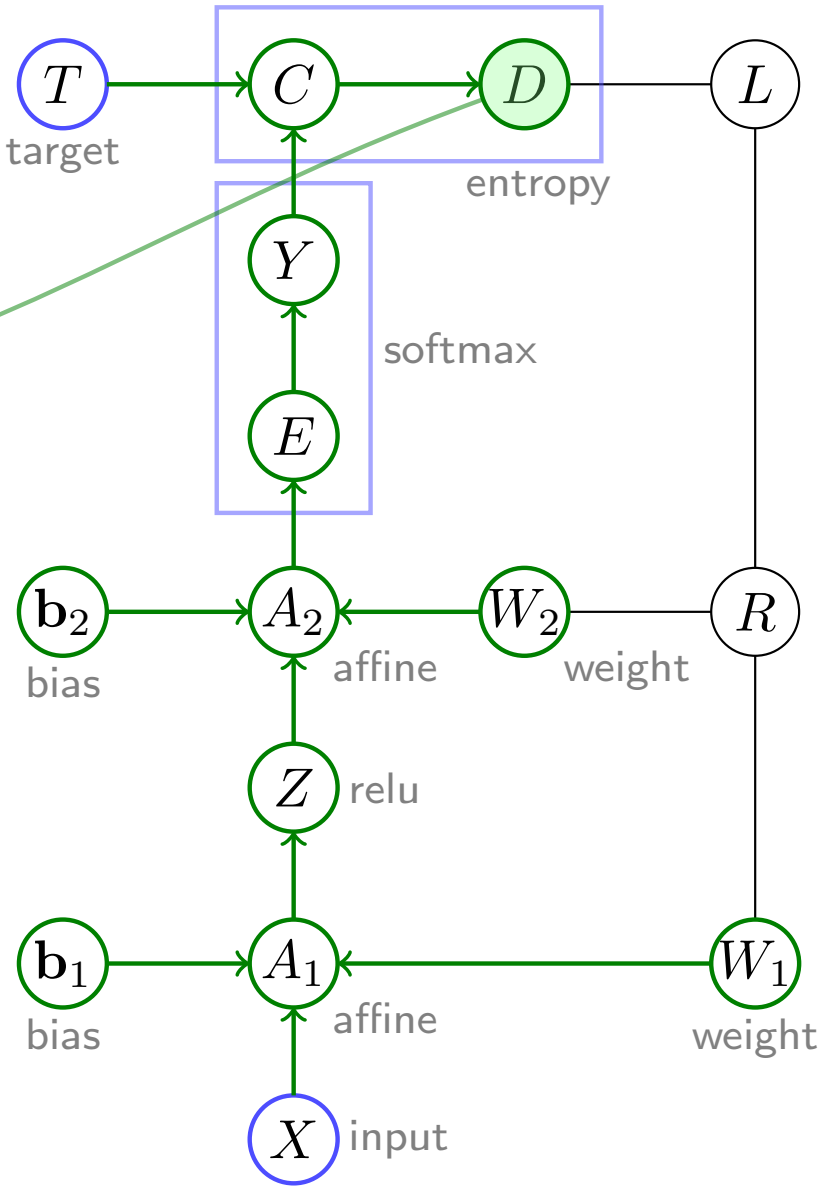

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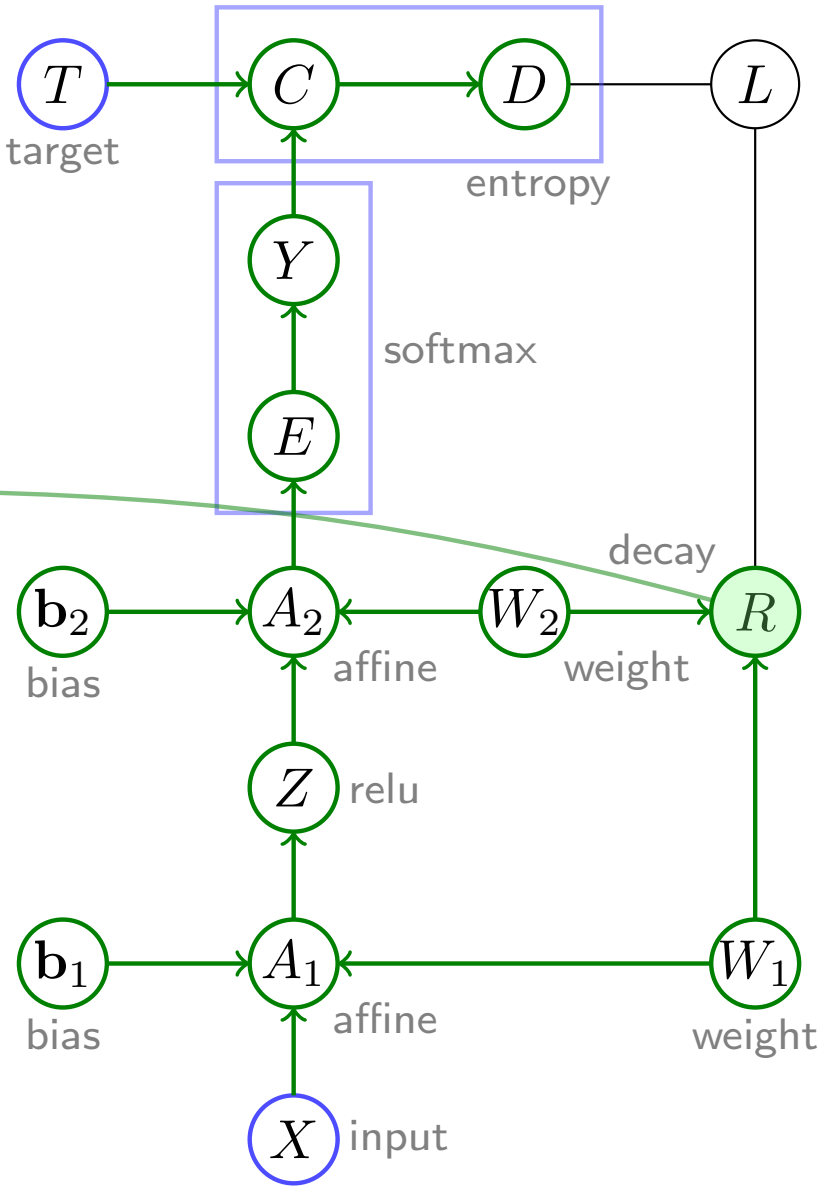
$$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$



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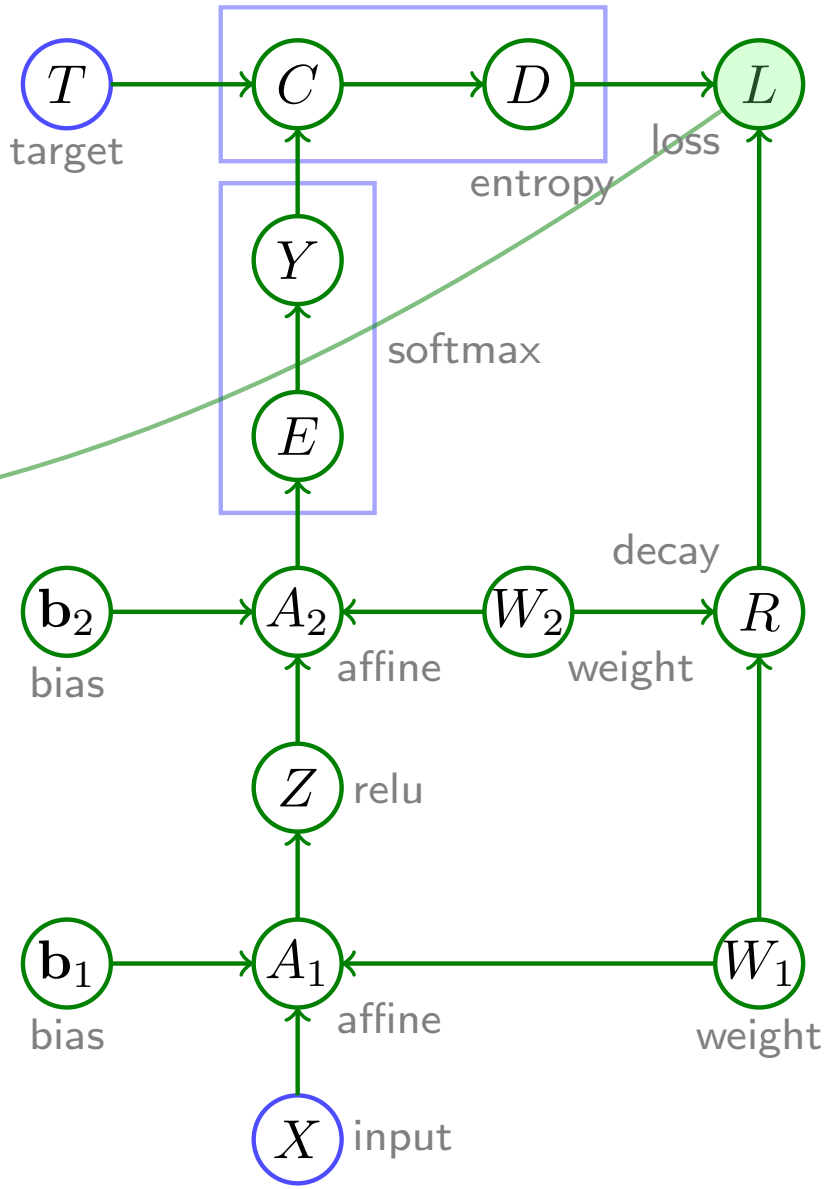
$$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$
$$\boxed{L = D + R}$$



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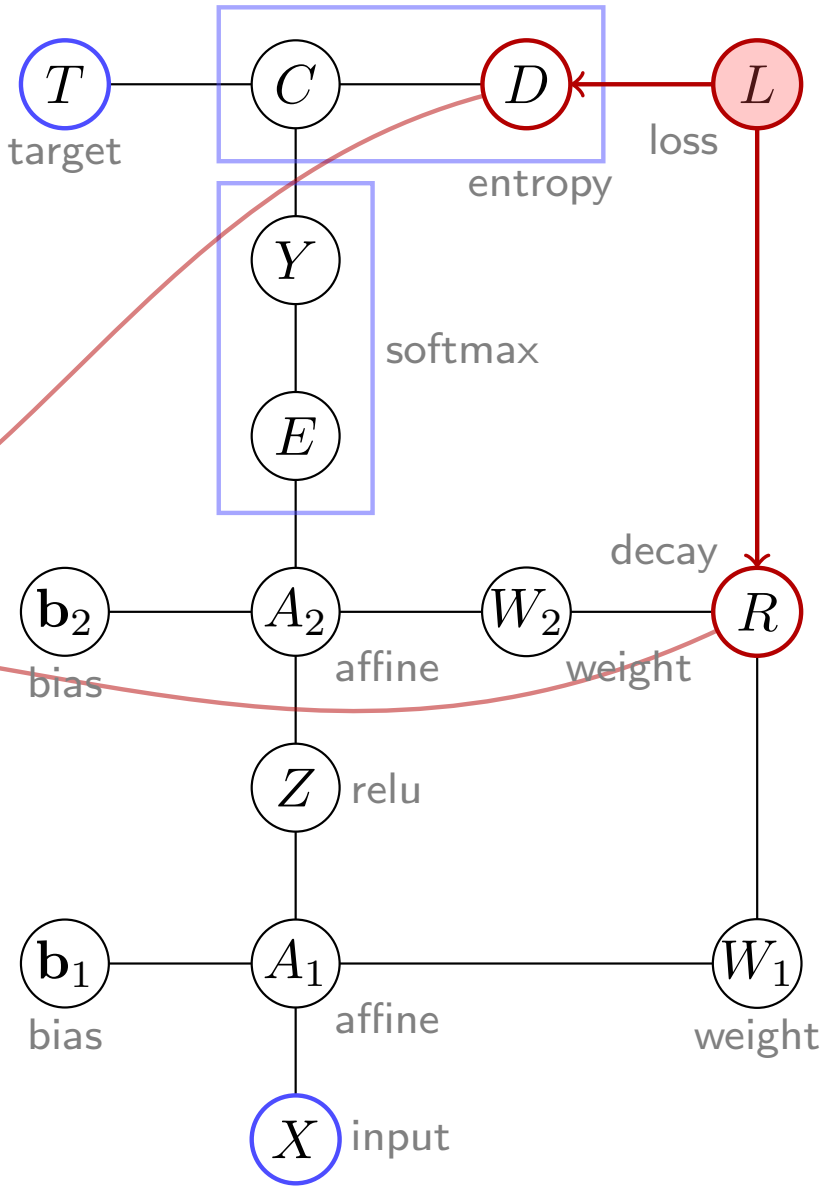
$$\boxed{(dD, dR) = (dL, dL)}$$



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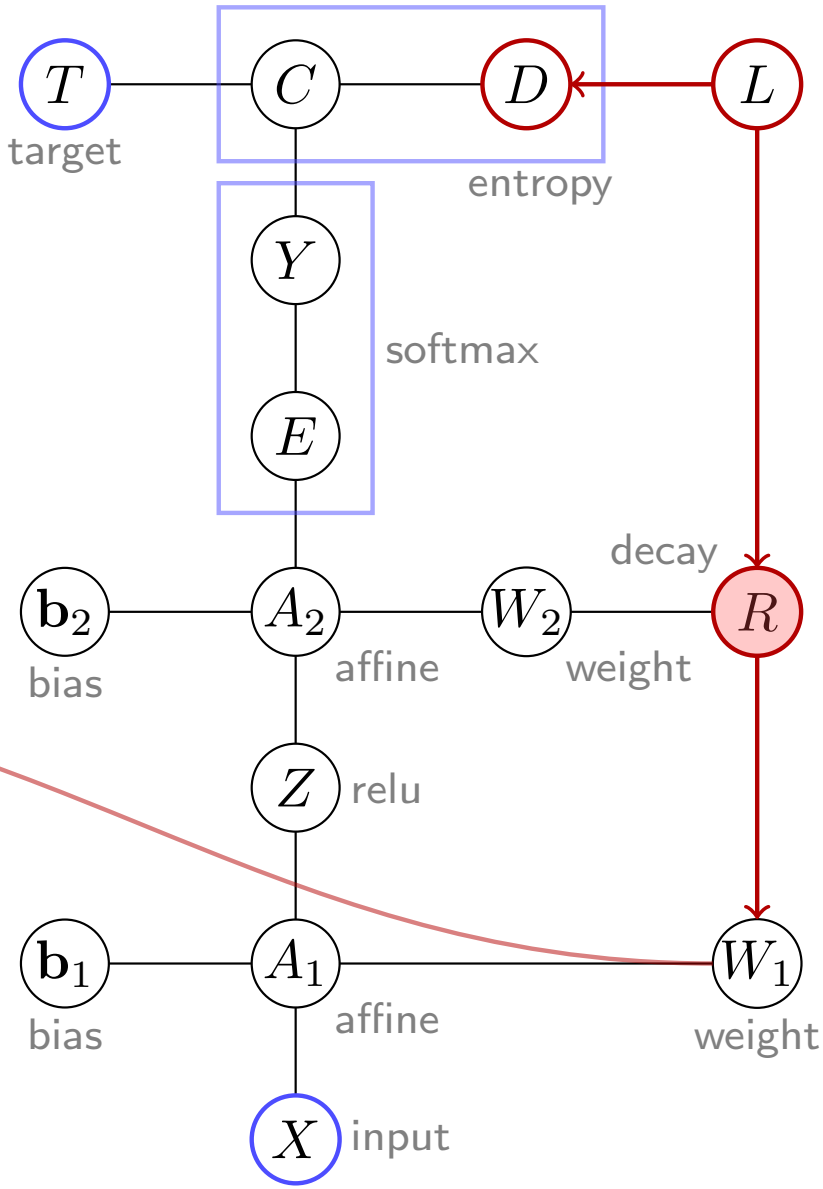
$$(dD, dR) = (dL, dL)$$
$$dW_1 = dR * \lambda * W_1$$
$$dW_2 = dR * \lambda * W_2$$



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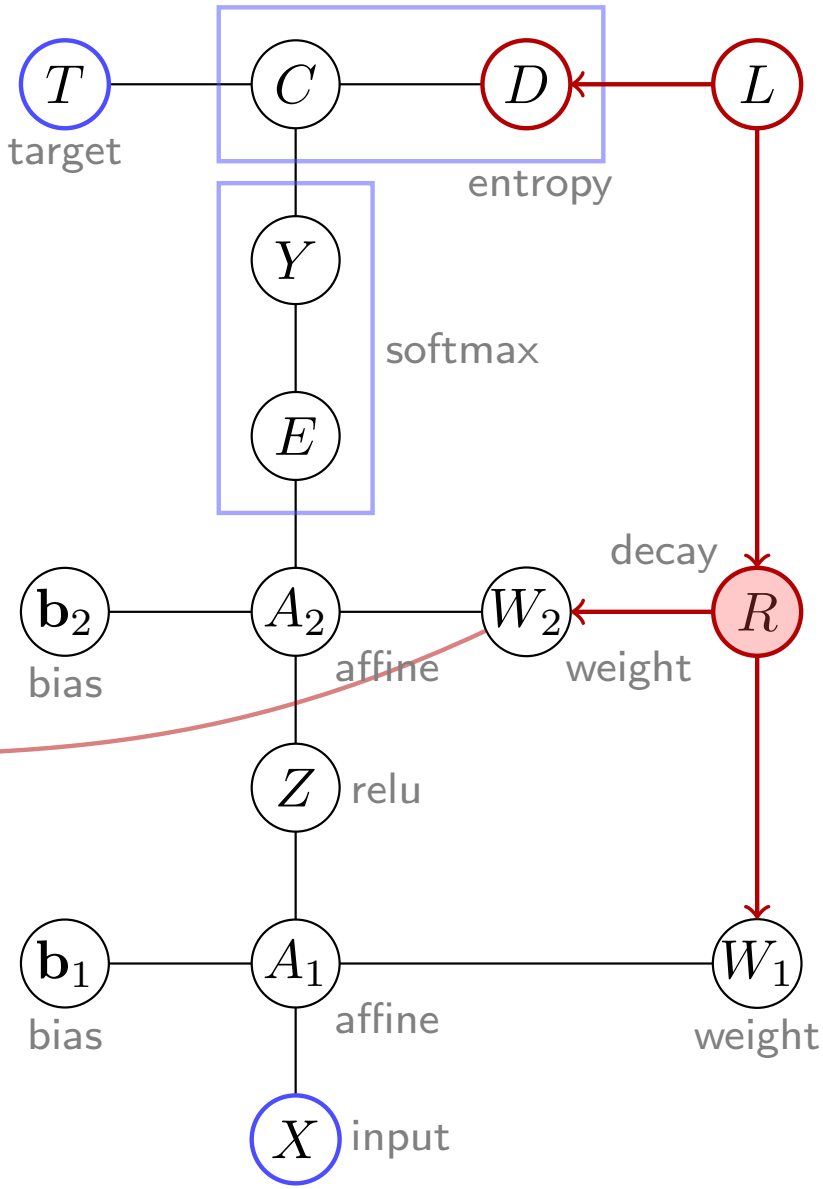

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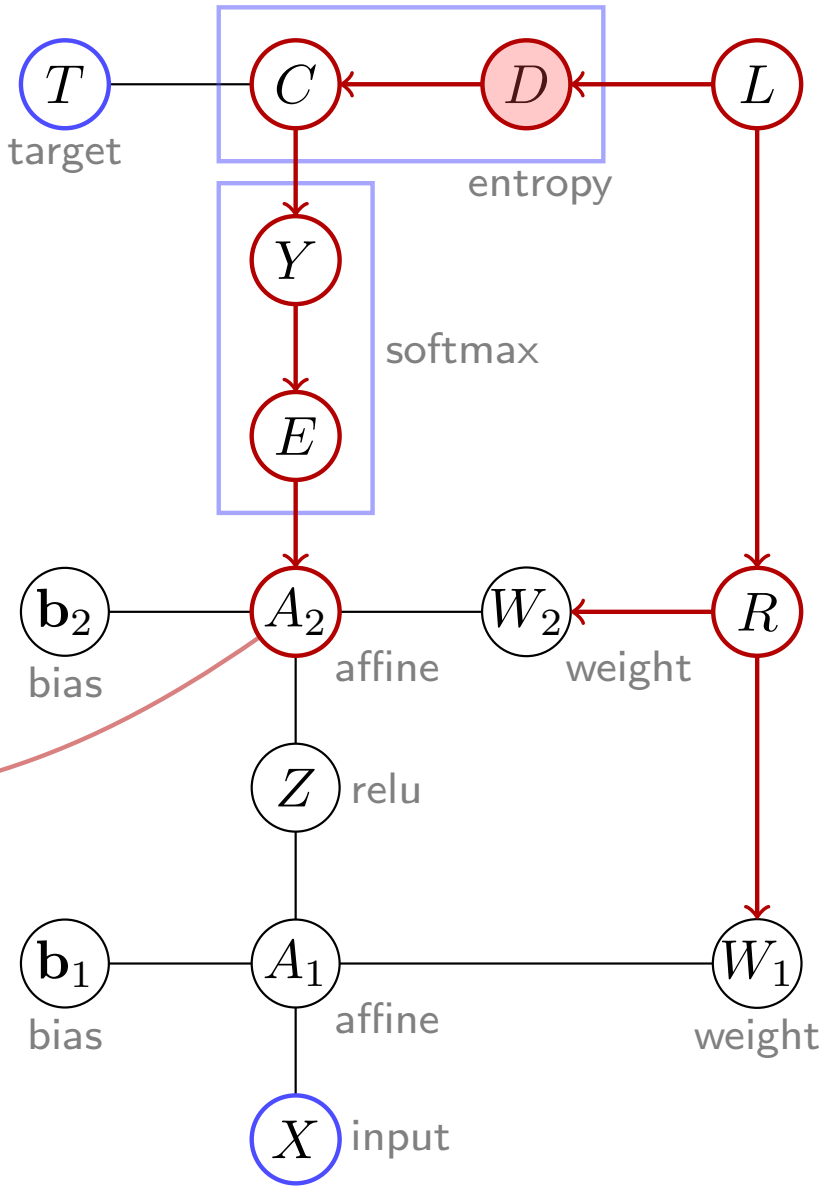
$$Z = \max(0, A_1)$$
$$A_2 = \mathrm{dot}(Z, W_2) + \mathbf{b}_2$$
$$E = \exp(A_2)$$
$$Y = E / \mathrm{sum}_1(E)$$
$$C = -\mathrm{sum}_1(T * \log(Y))$$
$$D = \mathrm{sum}_0(C)/m$$
$$R = \tfrac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$
$$L = D + R$$
$$(dD, dR) = (dL, dL)$$
$$dW_1 = dR * \lambda * W_1$$
$$dW_2 = dR * \lambda * W_2$$
$$\boxed{dA_2 = dD * (Y - T)/m}$$



back-propagation

$$A_1 = \mathrm{dot}(X, W_1) + \mathbf{b}_1$$
$$Z = \max(0, A_1)$$
$$A_2 = \mathrm{dot}(Z, W_2) + \mathbf{b}_2$$
$$E = \exp(A_2)$$
$$Y = E / \mathrm{sum}_1(E)$$
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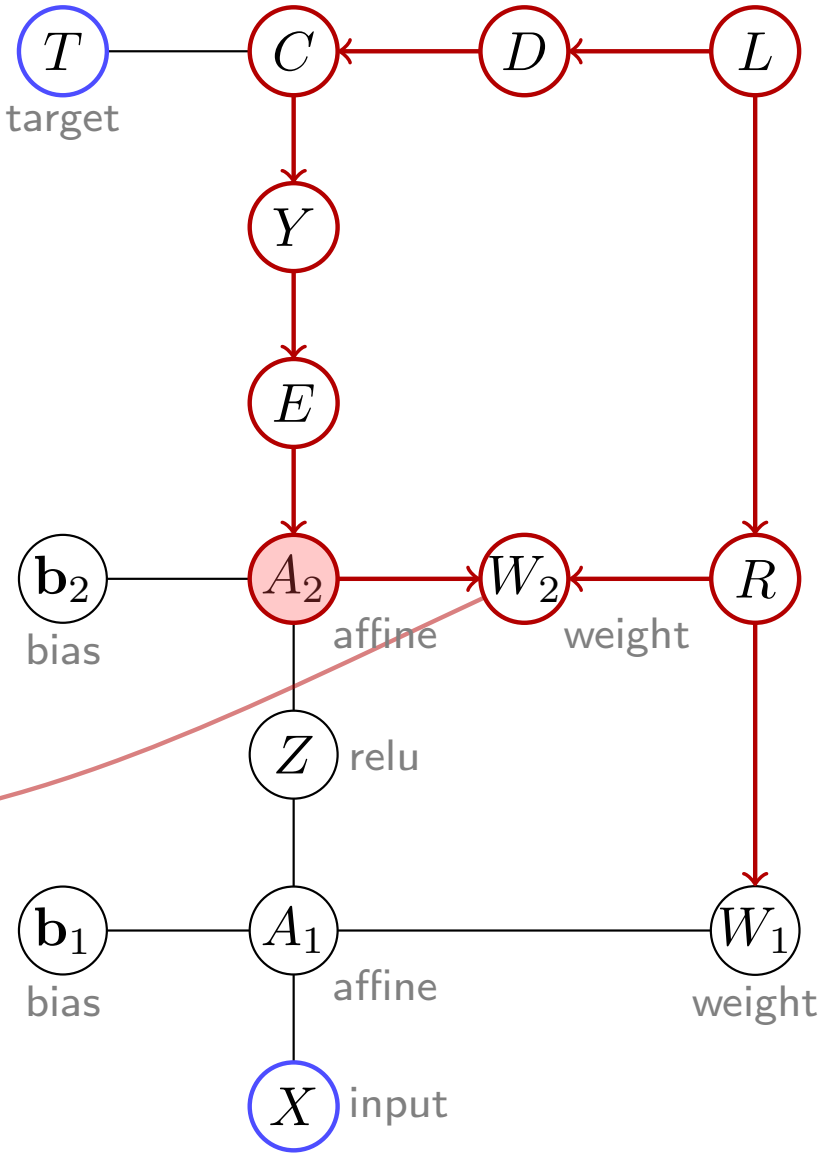
$$D = \mathrm{sum}_0(C)/m$$
$$R = \tfrac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$
$$L = D + R$$
$$(dD, dR) = (dL, dL)$$
$$dW_1 = dR * \lambda * W_1$$
$$dW_2 = dR * \lambda * W_2$$
$$dA_2 = dD * (Y - T)/m$$
$$dW_2 \mathrel{+}= \mathrm{dot}(Z^\top, dA_2)$$
$$d\mathbf{b}_2 = \mathrm{sum}_0(dA_2)$$
$$dZ = \mathrm{dot}(dA_2, W_2^\top)$$



back-propagation

$$A_1 = \mathrm{dot}(X, W_1) + \mathbf{b}_1$$
$$Z = \max(0, A_1)$$
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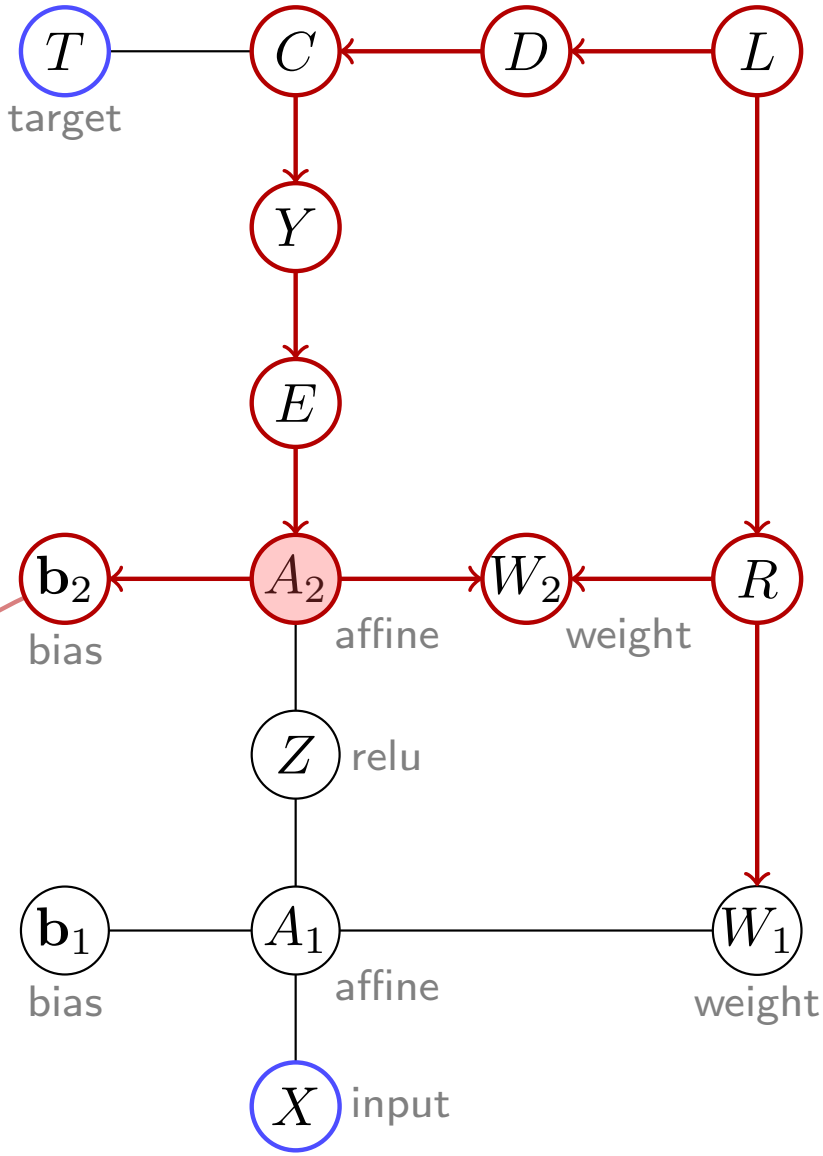
$$dA_2 = dD * (Y - T)/m$$
$$dW_2 \mathrel{+}= \mathrm{dot}(Z^\top, dA_2)$$
$$d\mathbf{b}_2 = \mathrm{sum}_0(dA_2)$$
$$dZ = \mathrm{dot}(dA_2, W_2^\top)$$



back-propagation

$$A_1 = \mathrm{dot}(X, W_1) + \mathbf{b}_1$$
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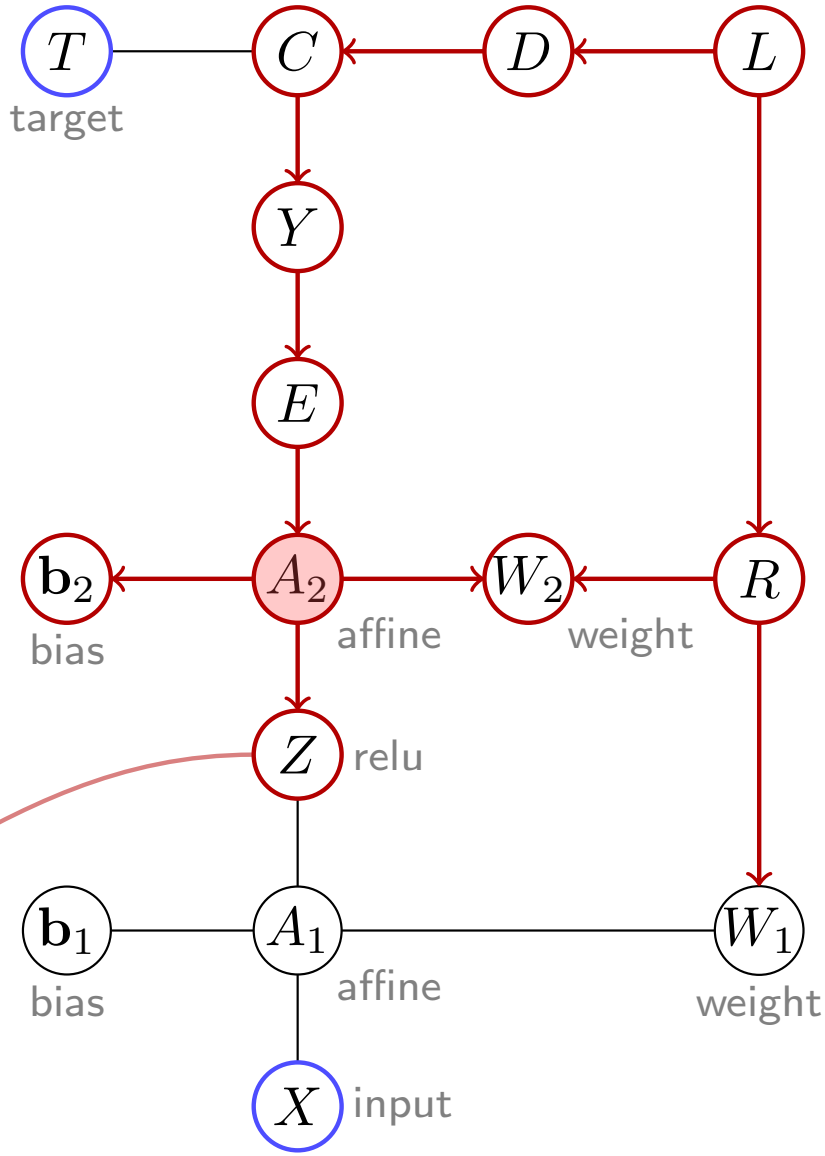
$$d\mathbf{b}_2 = \mathrm{sum}_0(dA_2)$$
$$dZ = \mathrm{dot}(dA_2, W_2^\top)$$



back-propagation

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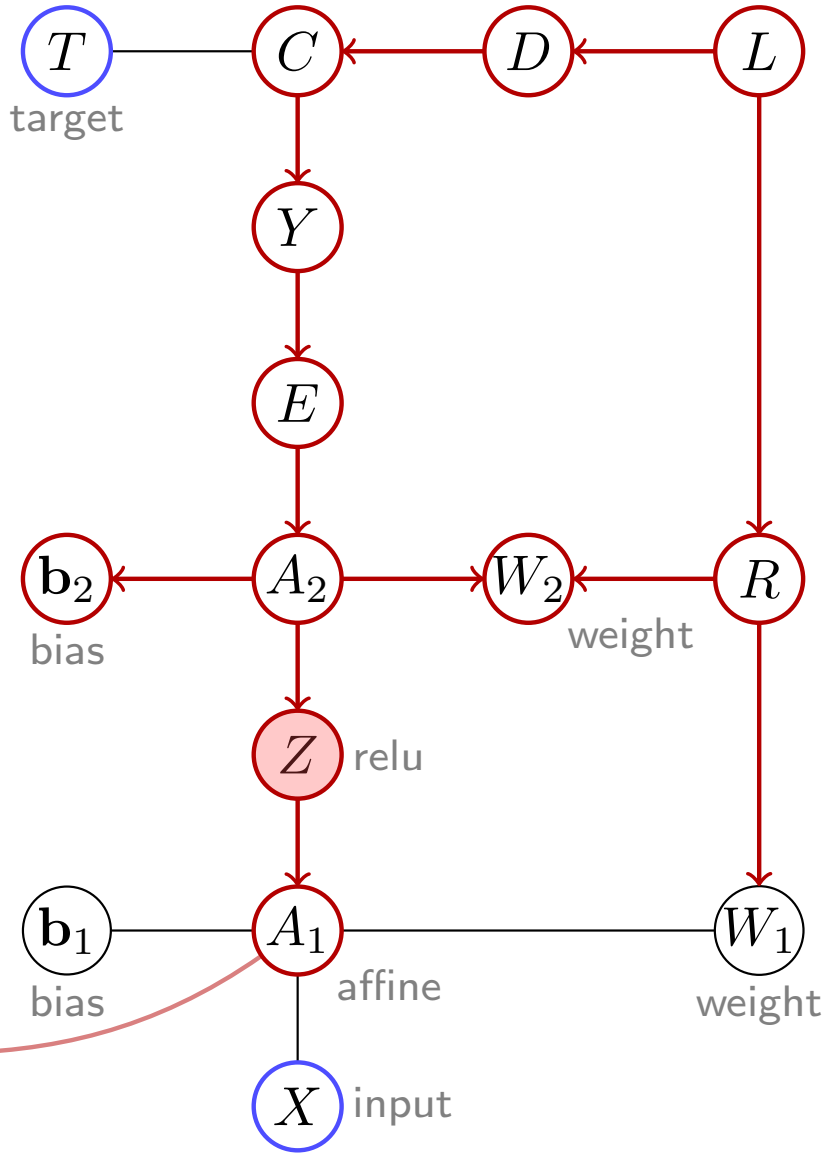
$$(dD, dR) = (dL, dL)$$
$$dW_1 = dR * \lambda * W_1$$
$$dW_2 = dR * \lambda * W_2$$
$$dA_2 = dD * (Y - T)/m$$
$$dW_2 \mathrel{+}= \text{dot}(Z^\top, dA_2)$$
$$d\mathbf{b}_2 = \text{sum}_0(dA_2)$$
$$dZ = \text{dot}(dA_2, W_2^\top)$$
$$dA_1 = dZ * (Z > 0)$$



back-propagation

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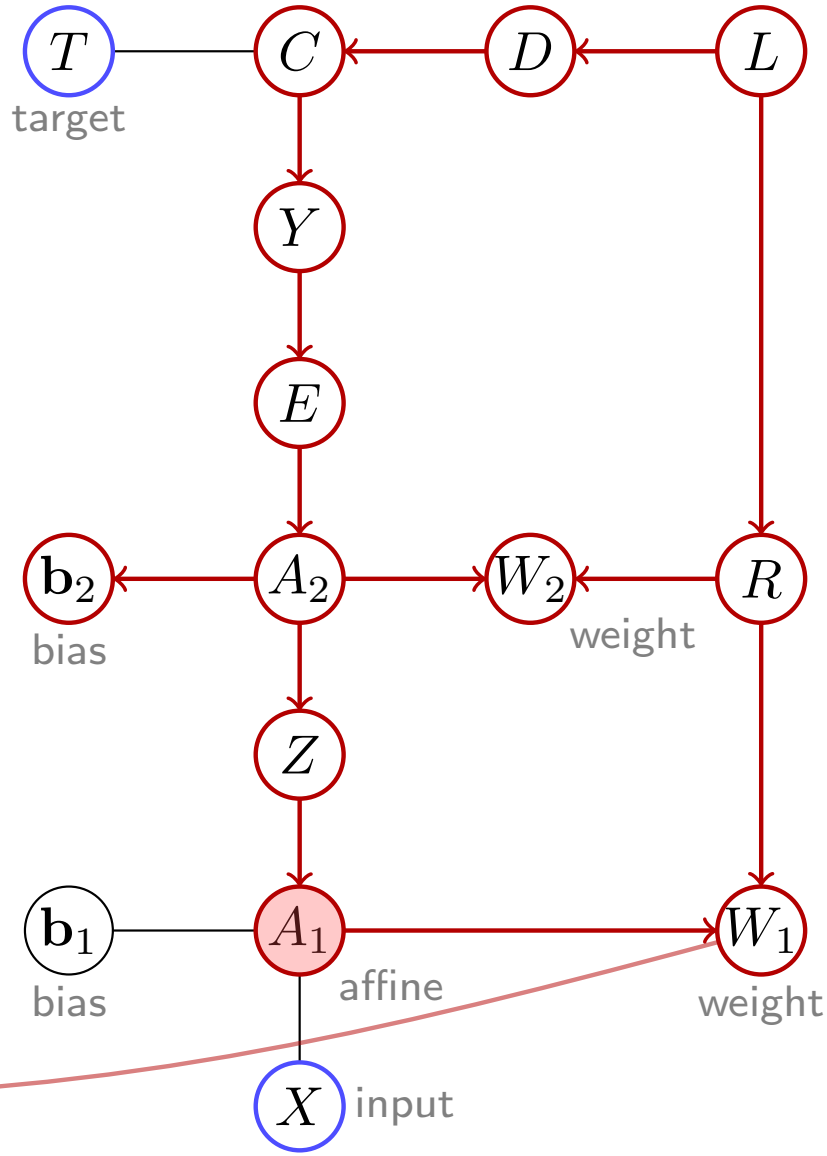
$$dA_2 = dD * (Y - T)/m$$
$$dW_2 \mathrel{+}= \text{dot}(Z^\top, dA_2)$$
$$d\mathbf{b}_2 = \text{sum}_0(dA_2)$$
$$dZ = \text{dot}(dA_2, W_2^\top)$$
$$dA_1 = dZ * (Z > 0)$$
$$dW_1 \mathrel{+}= \text{dot}(X^\top, dA_1)$$
$$d\mathbf{b}_1 = \text{sum}_0(dA_1)$$



back-propagation

$$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$$
$$Z = \max(0, A_1)$$
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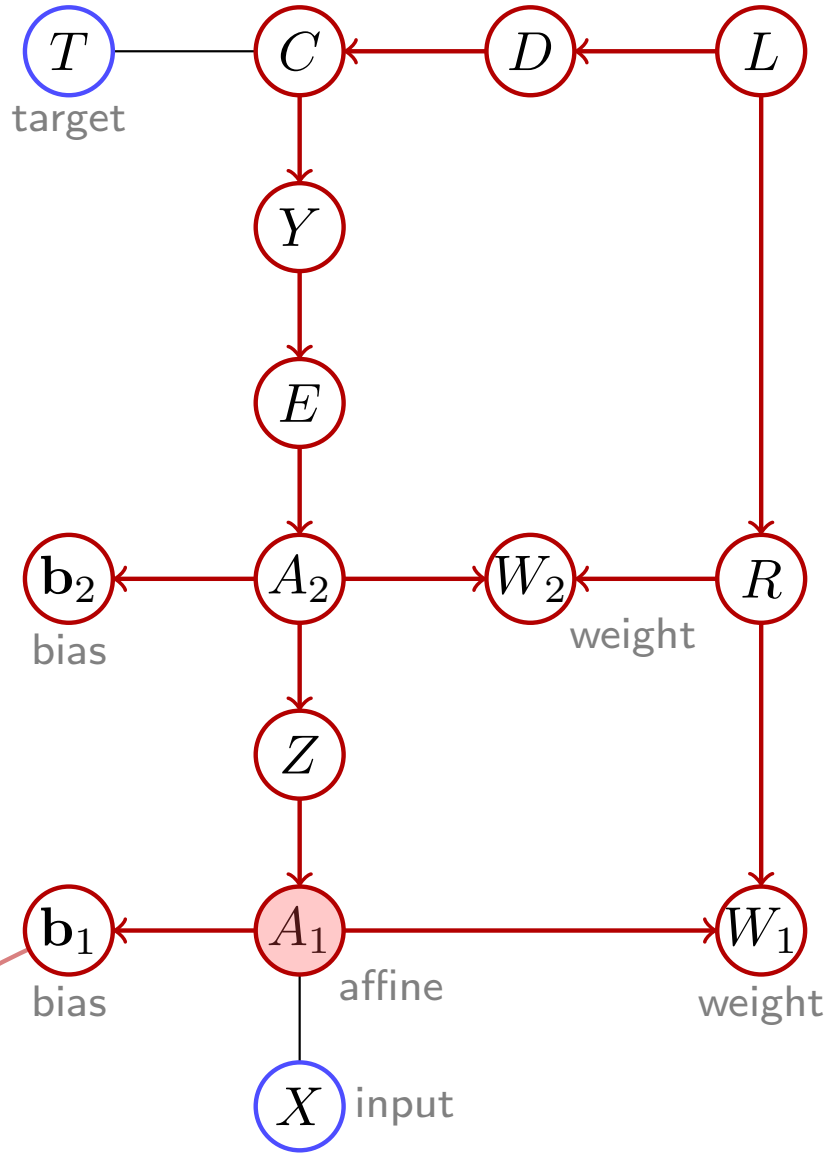
$$C = -\text{sum}_1(T * \log(Y))$$
$$D = \text{sum}_0(C)/m$$
$$R = \tfrac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$
$$L = D + R$$
$$(dD, dR) = (dL, dL)$$
$$dW_1 = dR * \lambda * W_1$$
$$dW_2 = dR * \lambda * W_2$$
$$dA_2 = dD * (Y - T)/m$$
$$dW_2 \mathrel{+}= \text{dot}(Z^\top, dA_2)$$
$$d\mathbf{b}_2 = \text{sum}_0(dA_2)$$
$$dZ = \text{dot}(dA_2, W_2^\top)$$
$$dA_1 = dZ * (Z > 0)$$
$$dW_1 \mathrel{+}= \text{dot}(X^\top, dA_1)$$
$$d\mathbf{b}_1 = \text{sum}_0(dA_1)$$



automatic differentiation

$$
\begin{aligned}
A_1 &= \mathrm{dot}(X, W_1) + \mathbf{b}_1 \\
Z &= \max(0, A_1) \\
A_2 &= \mathrm{dot}(Z, W_2) + \mathbf{b}_2 \\
E &= \exp(A_2) \\
Y &= E / \mathrm{sum}_1(E) \\
C &= -\mathrm{sum}_1(T * \log(Y)) \\
D &= \mathrm{sum}_0(C)/m \\
R &= \tfrac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2) \\
L &= D + R
\end{aligned}
$$

$$
\begin{aligned}
(dD, dR) &= (dL, dL) \\
dW_1 &= dR * \lambda * W_1 \\
dW_2 &= dR * \lambda * W_2 \\
dA_2 &= dD * (Y - T)/m \\
dW_2 &+= \mathrm{dot}(Z^\top, dA_2) \\
d\mathbf{b}_2 &= \mathrm{sum}_0(dA_2) \\
dZ &= \mathrm{dot}(dA_2, W_2^\top) \\
dA_1 &= dZ * (Z > 0) \\
dW_1 &+= \mathrm{dot}(X^\top, dA_1) \\
d\mathbf{b}_1 &= \mathrm{sum}_0(dA_1)
\end{aligned}
$$

now we organize forward and backward code into units and functions

automatic differentiation

$$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$$
$$Z = \max(0, A_1)$$
$$A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2$$
$$E = \exp(A_2)$$
$$Y = E / \text{sum}_1(E)$$
$$C = -\text{sum}_1(T * \log(Y))$$
$$D = \text{sum}_0(C)/m$$
$$R = \tfrac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$
$$L = D + R$$
$$(dD, dR) = (dL, dL)$$
$$dW_1 = dR * \lambda * W_1$$
$$dW_2 = dR * \lambda * W_2$$
$$dA_2 = dD * (Y - T)/m$$
$$dW_2 \mathrel{+}= \text{dot}(Z^\top, dA_2)$$
$$d\mathbf{b}_2 = \text{sum}_0(dA_2)$$
$$dZ = \text{dot}(dA_2, W_2^\top)$$
$$dA_1 = dZ * (Z > 0)$$
$$dW_1 \mathrel{+}= \text{dot}(X^\top, dA_1)$$
$$d\mathbf{b}_1 = \text{sum}_0(dA_1)$$

def relu(A):
  $Z = \max(0, A)$
  def back(dZ, dA):
    $dA \mathrel{+}= dZ * (Z > 0)$
  return $node(Z, \text{back})$

automatic differentiation

$$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$$
$$Z = \text{relu}(A_1)$$
$$A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2$$
$$E = \exp(A_2)$$
$$Y = E/\text{sum}_1(E)$$
$$C = -\text{sum}_1(T * \log(Y))$$
$$D = \text{sum}_0(C)/m$$
$$R = \tfrac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$
$$L = D + R$$
$$(dD, dR) = (dL, dL)$$
$$dW_1 = dR * \lambda * W_1$$
$$dW_2 = dR * \lambda * W_2$$
$$dA_2 = dD * (Y - T)/m$$
$$dW_2 \mathrel{+}= \text{dot}(Z^\top, dA_2)$$
$$d\mathbf{b}_2 = \text{sum}_0(dA_2)$$
$$dZ = \text{dot}(dA_2, W_2^\top)$$
$$Z.\text{back}(A_1)$$
$$dW_1 \mathrel{+}= \text{dot}(X^\top, dA_1)$$
$$d\mathbf{b}_1 = \text{sum}_0(dA_1)$$

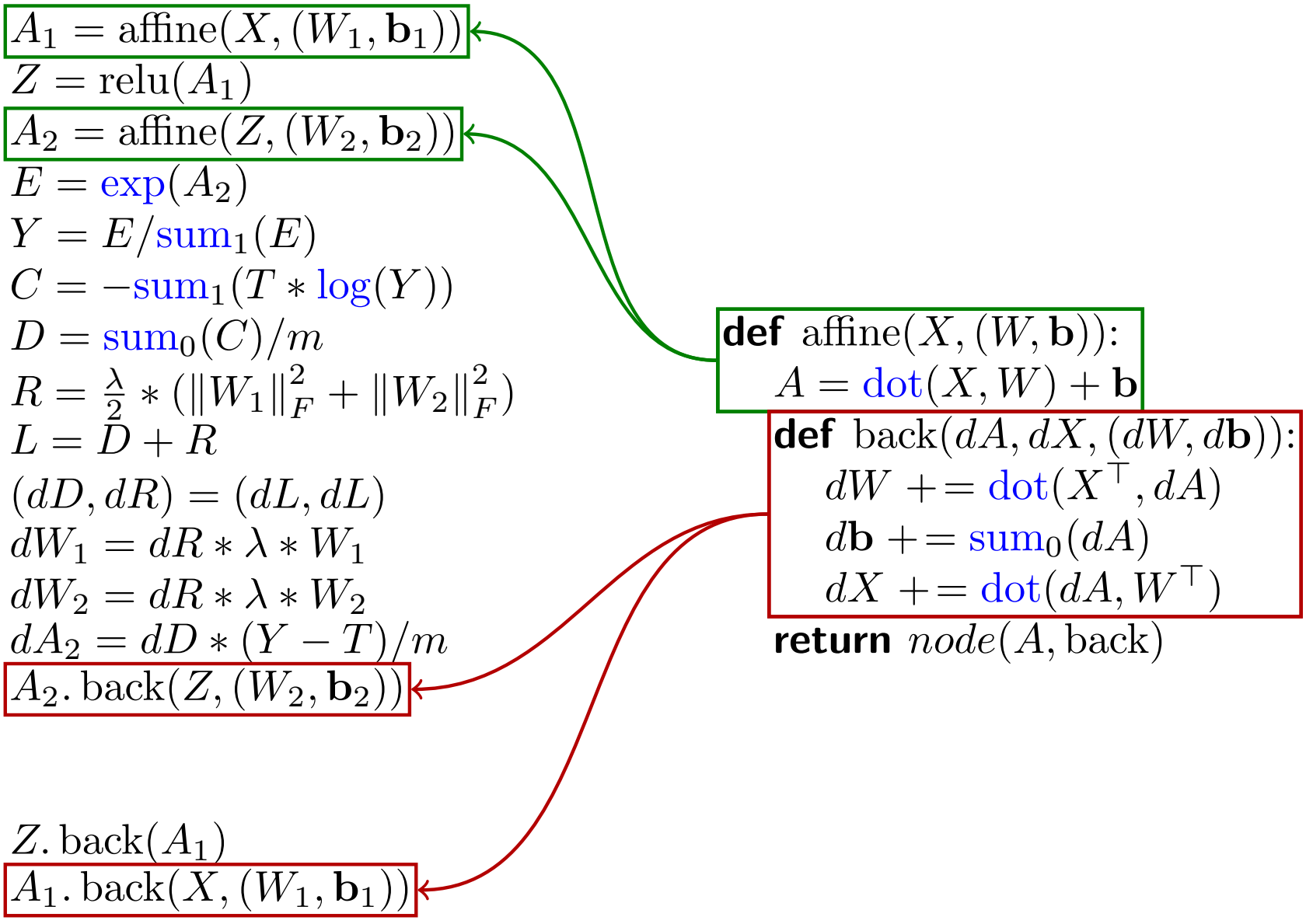
def relu(A):
    $Z = \max(0, A)$
    def back(dZ, dA):
        $dA \mathrel{+}= dZ * (Z > 0)$
    return $node(Z, \text{back})$

automatic differentiation

$A_1 = \mathrm{dot}(X, W_1) + \mathbf{b}_1$
$Z = \mathrm{relu}(A_1)$
$A_2 = \mathrm{dot}(Z, W_2) + \mathbf{b}_2$
$E = \exp(A_2)$
$Y = E/\mathrm{sum}_1(E)$
$C = -\mathrm{sum}_1(T * \log(Y))$
$D = \mathrm{sum}_0(C)/m$
$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$
$L = D + R$
$(dD, dR) = (dL, dL)$
$dW_1 = dR * \lambda * W_1$
$dW_2 = dR * \lambda * W_2$
$dA_2 = dD * (Y - T)/m$
$dW_2 \mathrel{+}= \mathrm{dot}(Z^\top, dA_2)$
$d\mathbf{b}_2 = \mathrm{sum}_0(dA_2)$
$dZ = \mathrm{dot}(dA_2, W_2^\top)$
$Z.\mathrm{back}(A_1)$
$dW_1 \mathrel{+}= \mathrm{dot}(X^\top, dA_1)$
$d\mathbf{b}_1 = \mathrm{sum}_0(dA_1)$

def affine$(X, (W, \mathbf{b}))$:
  $A = \mathrm{dot}(X, W) + \mathbf{b}$
  def back$(dA, dX, (dW, d\mathbf{b}))$:
    $dW \mathrel{+}= \mathrm{dot}(X^\top, dA)$
    $d\mathbf{b} \mathrel{+}= \mathrm{sum}_0(dA)$
    $dX \mathrel{+}= \mathrm{dot}(dA, W^\top)$
  return $node(A, \mathrm{back})$

automatic differentiation



automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$E = \exp(A_2)$
$Y = E/\text{sum}_1(E)$
$C = -\text{sum}_1(T * \log(Y))$
$D = \text{sum}_0(C)/m$
$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$
$L = D + R$
$(dD, dR) = (dL, dL)$
$dW_1 = dR * \lambda * W_1$
$dW_2 = dR * \lambda * W_2$
$dA_2 = dD * (Y - T)/m$
$A_2.\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\text{back}(A_1)$
$A_1.\text{back}(X, (W_1, \mathbf{b}_1))$

def logistic(A, T):
  $E = \exp(A)$
  $Y = E/\text{sum}_1(E)$
  $C = -\text{sum}_1(T * \log(Y))$
  $D = \text{sum}_0(C)/m$
  def back$(dD, dA, _)$:
    $dA \mathrel{+}= dD * (Y - T)/m$
  return $node(D, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$D = \text{logistic}(A_2, T)$

$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$
$L = D + R$
$(dD, dR) = (dL, dL)$
$dW_1 = dR * \lambda * W_1$
$dW_2 = dR * \lambda * W_2$
$D.\text{back}(A_2, T)$
$A_2.\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\text{back}(A_1)$
$A_1.\text{back}(X, (W_1, \mathbf{b}_1))$

def logistic(A, T):
    $E = \exp(A)$
    $Y = E/\text{sum}_1(E)$
    $C = -\text{sum}_1(T * \log(Y))$
    $D = \text{sum}_0(C)/m$
    def back$(dD, dA, _)$:
        $dA \mathrel{+}= dD * (Y - T)/m$
    return $node(D, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$D = \text{logistic}(A_2, T)$

$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$
$L = D + R$
$(dD, dR) = (dL, dL)$
$dW_1 = dR * \lambda * W_1$
$dW_2 = dR * \lambda * W_2$
$D.\text{back}(A_2, T)$
$A_2.\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\text{back}(A_1)$
$A_1.\text{back}(X, (W_1, \mathbf{b}_1))$

def decay(W):
  $R = \frac{\lambda}{2} * \text{sum}(\|w\|_F^2$ **for** w **in** $W)$
def back(dR, dW):
  for (w, dw) **in** zip(W, dW):
    $dw \mathrel{+}= dR * \lambda * w$
return $node(R, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$D = \text{logistic}(A_2, T)$

$R = \text{decay}((W_1, W_2))$
$L = D + R$
$(dD, dR) = (dL, dL)$
$R.\,\text{back}((W_1, W_2))$

$D.\,\text{back}(A_2, T)$
$A_2.\,\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\,\text{back}(A_1)$
$A_1.\,\text{back}(X, (W_1, \mathbf{b}_1))$

def decay(W):
    $R = \frac{\lambda}{2} * \text{sum}(\|w\|_F^2$ **for** w **in** $W)$
    def back(dR, dW):
        for (w, dw) **in** zip(W, dW):
            $dw \mathrel{+}= dR * \lambda * w$
    return $node(R, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$D = \text{logistic}(A_2, T)$

$R = \text{decay}((W_1, W_2))$
$L = D + R$
$(dD, dR) = (dL, dL)$
$R.\,\text{back}((W_1, W_2))$

$D.\,\text{back}(A_2, T)$
$A_2.\,\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\,\text{back}(A_1)$
$A_1.\,\text{back}(X, (W_1, \mathbf{b}_1))$

def add(X):
  $S = \text{sum}(X)$
  def back(dS, dX):
    for dx **in** dX:
      $dx \mathrel{+}= dS$
  return $node(S, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$D = \text{logistic}(A_2, T)$

$R = \text{decay}((W_1, W_2))$
$L = \text{add}((D, R))$
$L.\,\text{back}((D, R))$
$R.\,\text{back}((W_1, W_2))$

$D.\,\text{back}(A_2, T)$
$A_2.\,\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\,\text{back}(A_1)$
$A_1.\,\text{back}(X, (W_1, \mathbf{b}_1))$

def $\text{add}(X)$:
    $S = \text{sum}(X)$
    def $\text{back}(dS, dX)$:
        for dx **in** dX:
            $dx \mathrel{+}= dS$
    return $node(S, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$D = \text{logistic}(A_2, T)$
$R = \text{decay}((W_1, W_2))$
$L = \text{add}((D, R))$
$L.\,\text{back}((D, R))$
$R.\,\text{back}((W_1, W_2))$
$D.\,\text{back}(A_2, T)$
$A_2.\,\text{back}(Z, (W_2, \mathbf{b}_2))$
$Z.\,\text{back}(A_1)$
$A_1.\,\text{back}(X, (W_1, \mathbf{b}_1))$

def $\text{loss}(A, T, W)$:
$D = \text{logistic}(A, T)$
$R = \text{decay}(W)$
$L = \text{add}((D, R))$
def $\text{back}(A, T, W)$:
$L.\,\text{back}((D, R))$
$R.\,\text{back}(W)$
$D.\,\text{back}(A, T)$
return $block(L, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$L = \text{loss}(A_2, T, (W_1, W_2))$

def $\text{loss}(A, T, W)$:
  $D = \text{logistic}(A, T)$
  $R = \text{decay}(W)$
  $L = \text{add}((D, R))$
  def $\text{back}(A, T, W)$:
    $L.\,\text{back}((D, R))$
    $R.\,\text{back}(W)$
    $D.\,\text{back}(A, T)$
  return $block(L, \text{back})$

$L.\,\text{back}(A_2, T, (W_1, W_2))$

$A_2.\,\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\,\text{back}(A_1)$
$A_1.\,\text{back}(X, (W_1, \mathbf{b}_1))$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$L = \text{loss}(A_2, T, (W_1, W_2))$

$L.\,\text{back}(A_2, T, (W_1, W_2))$

$A_2.\,\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\,\text{back}(A_1)$
$A_1.\,\text{back}(X, (W_1, \mathbf{b}_1))$

def $\text{loss}(A, T, W)$:
    $L = \text{logistic}(A, T) + \text{decay}(W)$
    return $block(L)$

def $\text{loss}(A, T, W)$:
    $D = \text{logistic}(A, T)$
    $R = \text{decay}(W)$
    $L = \text{add}((D, R))$
    def $\text{back}(A, T, W)$:
        $L.\,\text{back}((D, R))$
        $R.\,\text{back}(W)$
        $D.\,\text{back}(A, T)$
    return $block(L, \text{back})$

automatic differentiation

$A_1 = \text{affine}(X, (W_1, \mathbf{b}_1))$
$Z = \text{relu}(A_1)$
$A_2 = \text{affine}(Z, (W_2, \mathbf{b}_2))$
$L = \text{loss}(A_2, T, (W_1, W_2))$

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$A_2.\,\text{back}(Z, (W_2, \mathbf{b}_2))$

$Z.\,\text{back}(A_1)$
$A_1.\,\text{back}(X, (W_1, \mathbf{b}_1))$

def $\text{model}(X, (U_1, U_2))$:
  $A_1 = \text{affine}(X, U_1)$
  $Z = \text{relu}(A)$
  $A_2 = \text{affine}(Z, U_2)$
  def $\text{back}(X, (U_1, U_2))$:
    $A_2.\,\text{back}(Z, U_2)$
    $Z.\,\text{back}(A)$
    $A_1.\,\text{back}(X, U_1)$
  return $block(A_2, \text{back})$

automatic differentiation

$A_2 = \text{model}(X, ((W_1, \mathbf{b}_1), (W_2, \mathbf{b}_2)))$

$L = \text{loss}(A_2, T, (W_1, W_2))$

$L.\text{back}(A_2, T, (W_1, W_2))$

$A_2.\text{back}(X, ((W_1, \mathbf{b}_1), (W_2, \mathbf{b}_2)))$

def $\text{model}(X, (U_1, U_2))$:
  $A_1 = \text{affine}(X, U_1)$
  $Z = \text{relu}(A)$
  $A_2 = \text{affine}(Z, U_2)$

def $\text{back}(X, (U_1, U_2))$:
  $A_2.\text{back}(Z, U_2)$
  $Z.\text{back}(A)$
  $A_1.\text{back}(X, U_1)$

return $block(A_2, \text{back})$

automatic differentiation

$A_2 = \text{model}(X, ((W_1, \mathbf{b}_1), (W_2, \mathbf{b}_2)))$

$L = \text{loss}(A_2, T, (W_1, W_2))$

$L.\,\text{back}(A_2, T, (W_1, W_2))$

$A_2.\,\text{back}(X, ((W_1, \mathbf{b}_1), (W_2, \mathbf{b}_2)))$

def $\text{model}(X, (U_1, U_2))$:
  $A = \text{affine}(\text{relu}(\text{affine}(X, U_1)), U_2)$
  return $block(A)$

def $\text{model}(X, (U_1, U_2))$:
  $A_1 = \text{affine}(X, U_1)$
  $Z = \text{relu}(A)$
  $A_2 = \text{affine}(Z, U_2)$
  def $\text{back}(X, (U_1, U_2))$:
    $A_2.\,\text{back}(Z, U_2)$
    $Z.\,\text{back}(A)$
    $A_1.\,\text{back}(X, U_1)$
  return $block(A_2, \text{back})$

what is not shown

- $units$s and $functions$s are actually objects
  - both expose a "call" operator $()$ for the forward pass, which handles recording of calls
  - $function$'s operator also generates method back and constructs a $block$ object for the backward pass
  - both expose method init, which handles initialization of parameters, if any

deep learning software

- automatically build computational graphs and compute derivatives
- run on GPU, multiple GPU, distributed
- component (unit, layer) libraries
- pre-trained models
- community

fun

CIFAR10 dataset

plane car bird cat deer dog frog horse ship truck

- 10 classes, 50k training images, 10k test images, 32×32 images

Krizhevsky and Hinton 2009. Learning Multiple Layers of Features From Tiny Images.

pipeline

prepare

- vectorize $32 \times 32 \times 3$ images into 3072×1
- split training set *e.g.* into $n_{\text{train}} = 45000$ training samples and $n_{\text{val}} = 5000$ samples to be used for validation
- center vectors by subtracting mean over the training samples
- initialize network weights as Gaussian with standard deviation 10^{-4}

learn

- train for a few iterations and evaluate accuracy on the validation set for a number of learning rates ϵ and regularization strengths λ
- train for 10 epochs on the full training set for the chosen hyperparameters
- evaluate accuracy on the test set

pipeline

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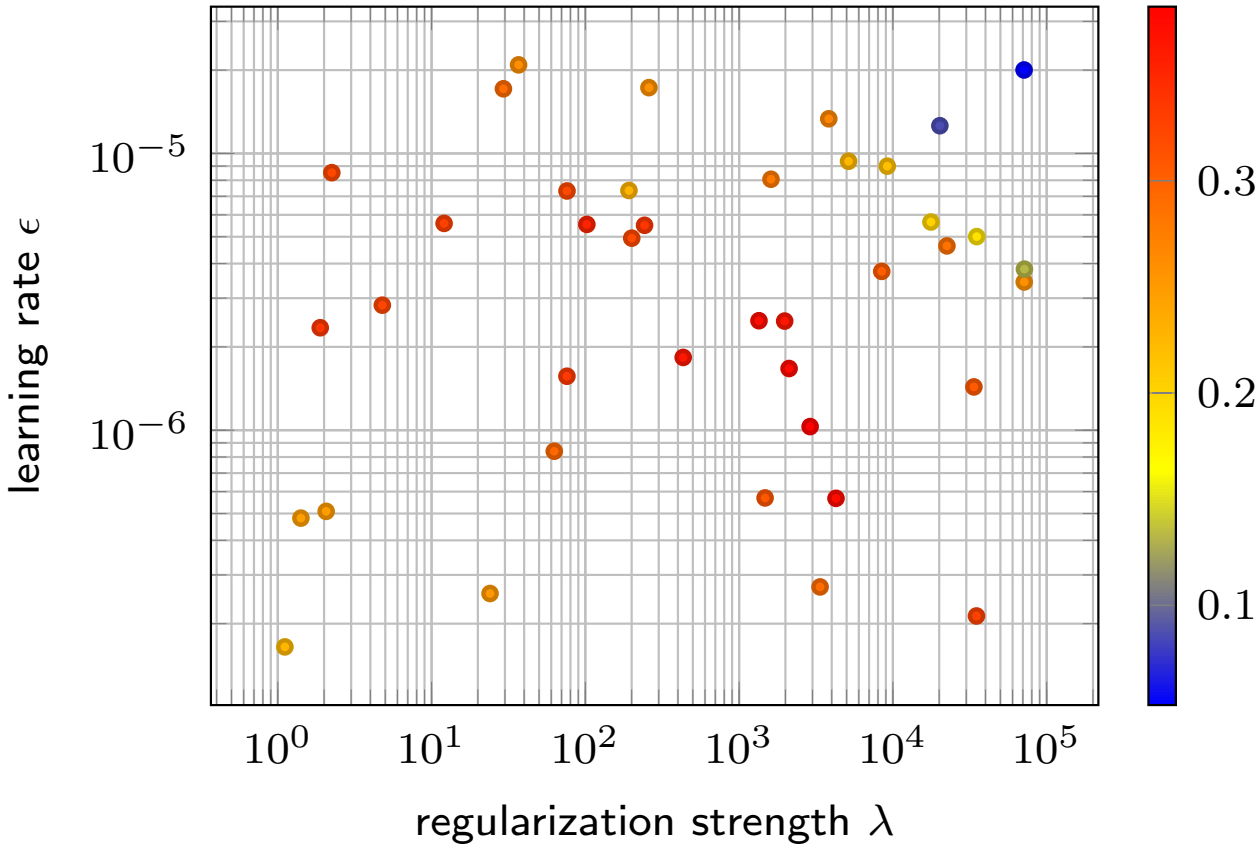
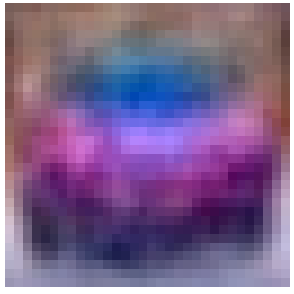
linear classifier validation accuracy



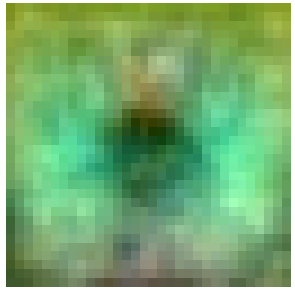
- classes $k = 10$, samples $n_{\text{train}} = 45000, n_{\text{val}} = 5000$, mini-batch $m = 200$, learning rate $\epsilon = 10^{-6}$, regularization strength $\lambda = 5 \times 10^2$
- test accuracy: 38%

linear classifier weights

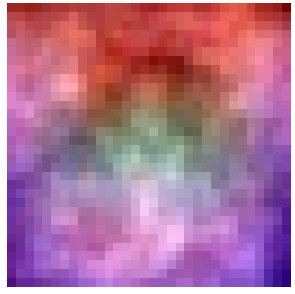
plane



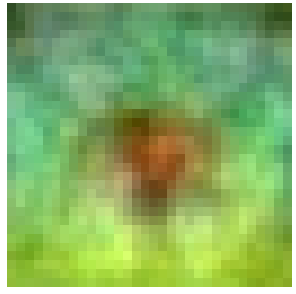
car



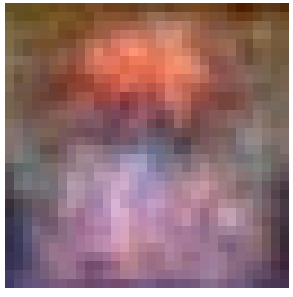
bird



cat



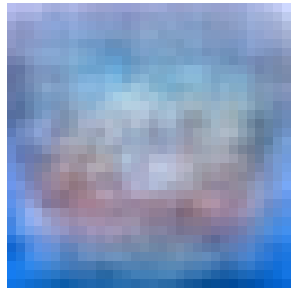
deer



dog

frog

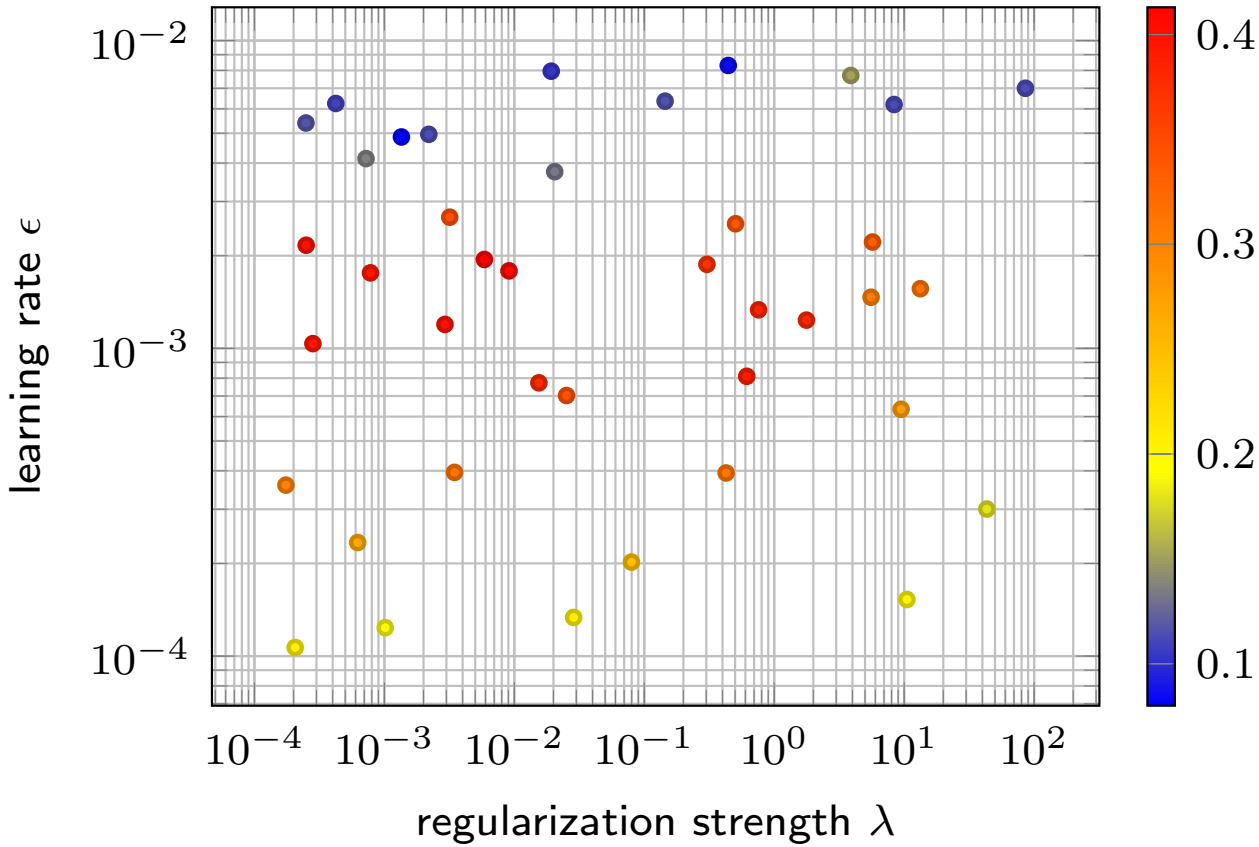
horse



ship

truck

2-layer classifier validation accuracy



- classes $k = 10$, samples $n_{\text{train}} = 45000, n_{\text{val}} = 5000$, mini-batch $m = 200$, learning rate $2 \times \epsilon = 10^{-3}$, regularization strength $\lambda = 2 \times 10^{-1}$
- hidden layer width: 100; test accuracy: 51%

two-layer classifier weights

layer 1 weights 0-49

two-layer classifier weights

layer 1 weights 50-99

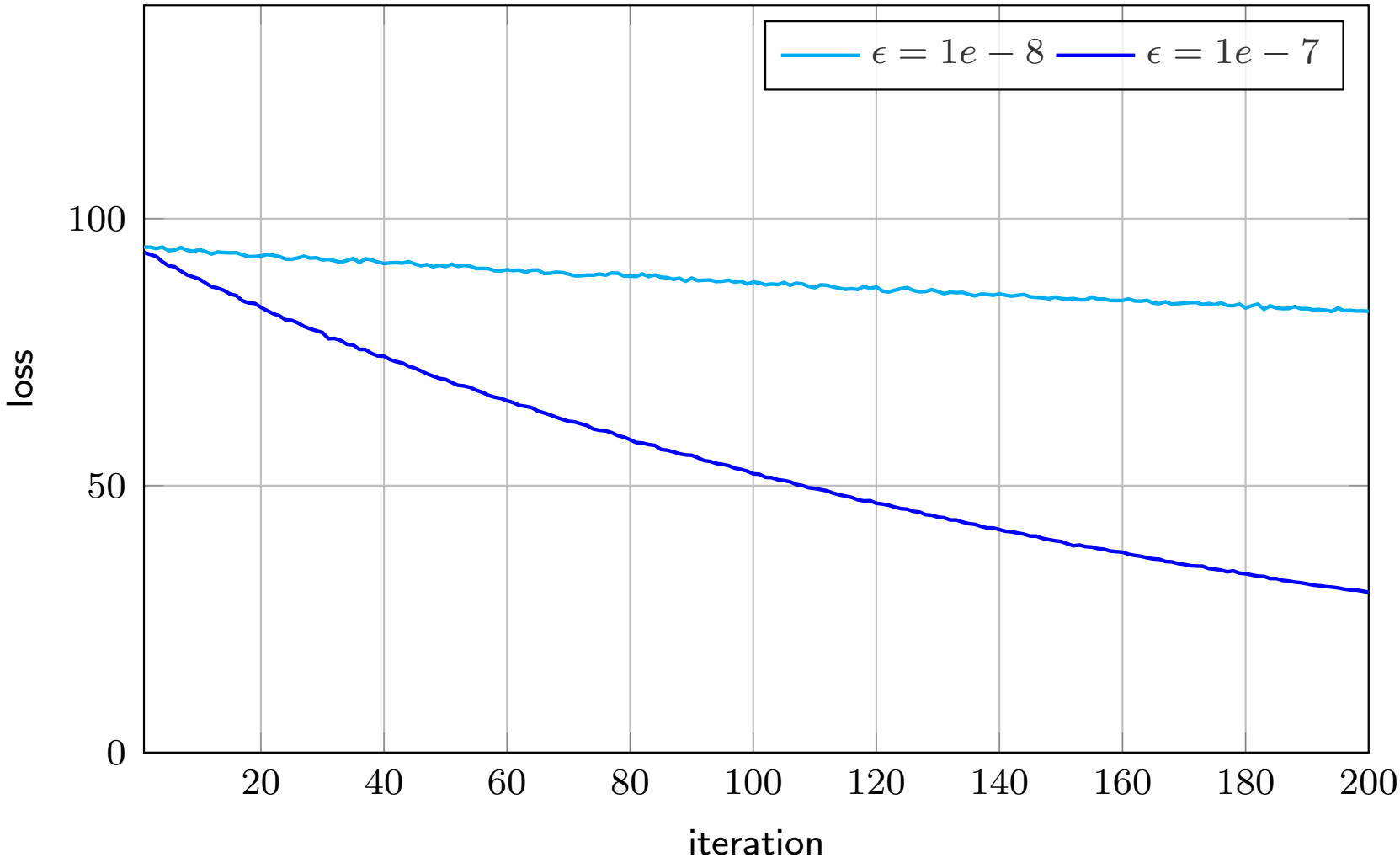
two-layer classifier weights

layer 1 weights 100-149

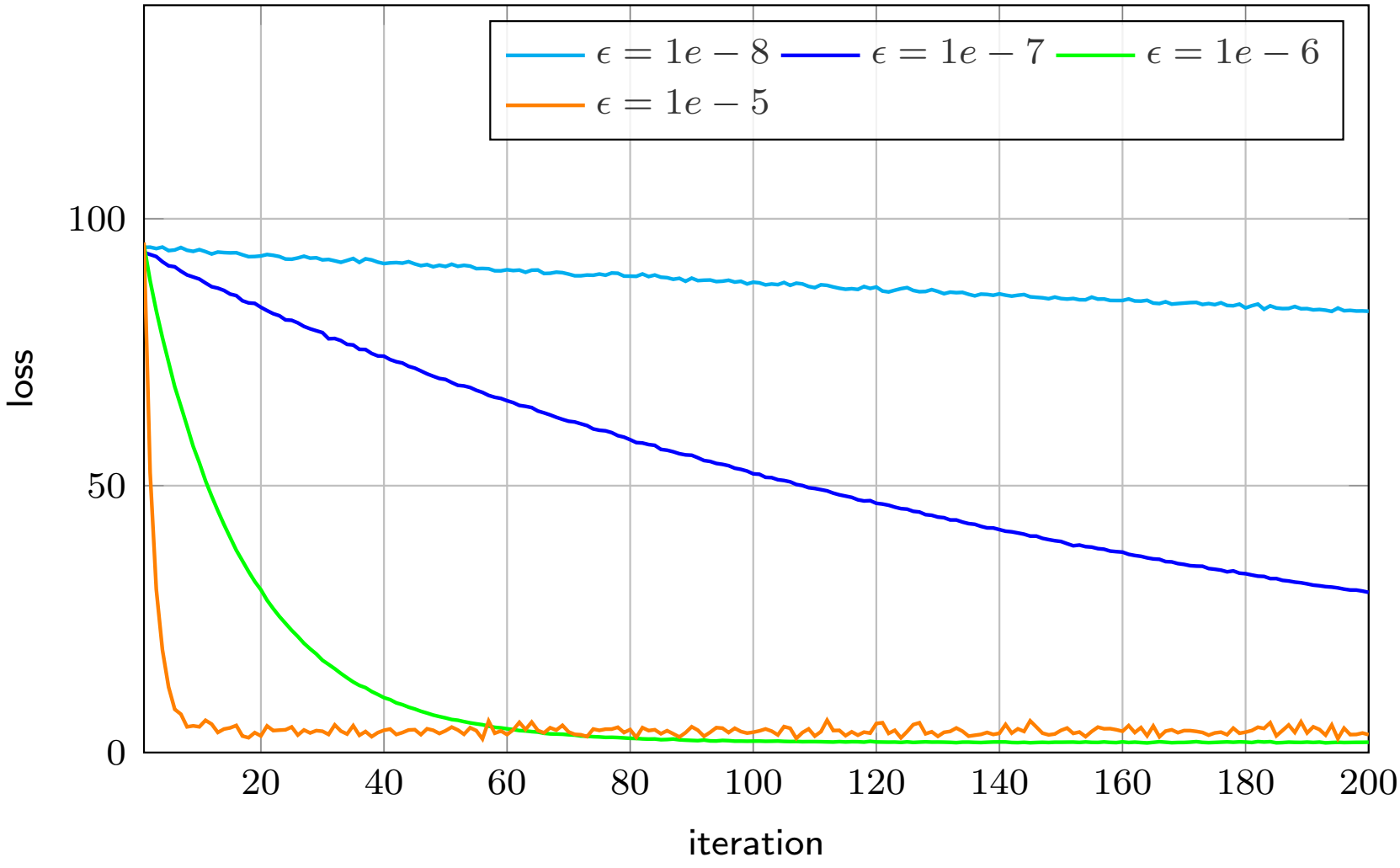
two-layer classifier weights

layer 1 weights 150-199

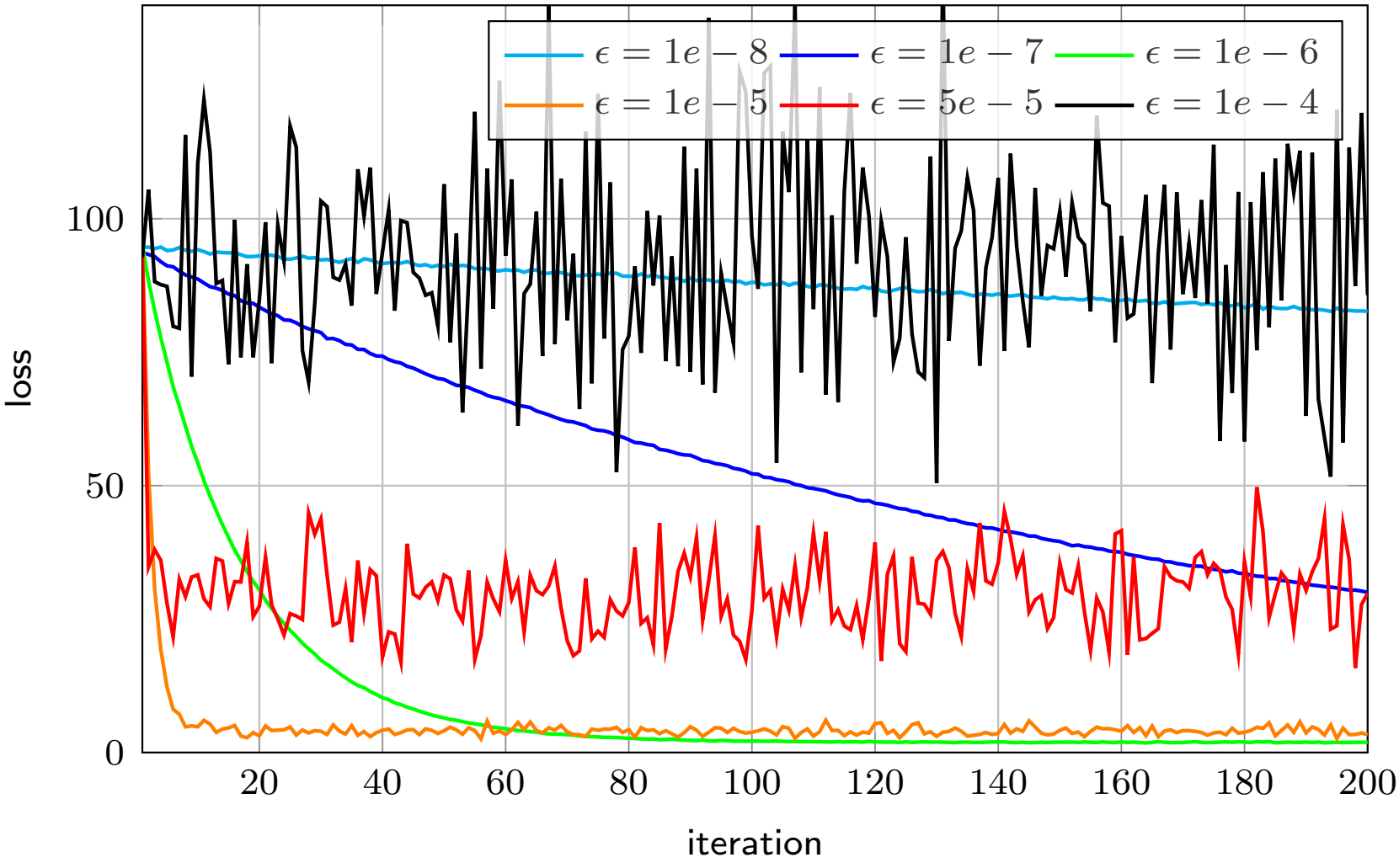
learning rate



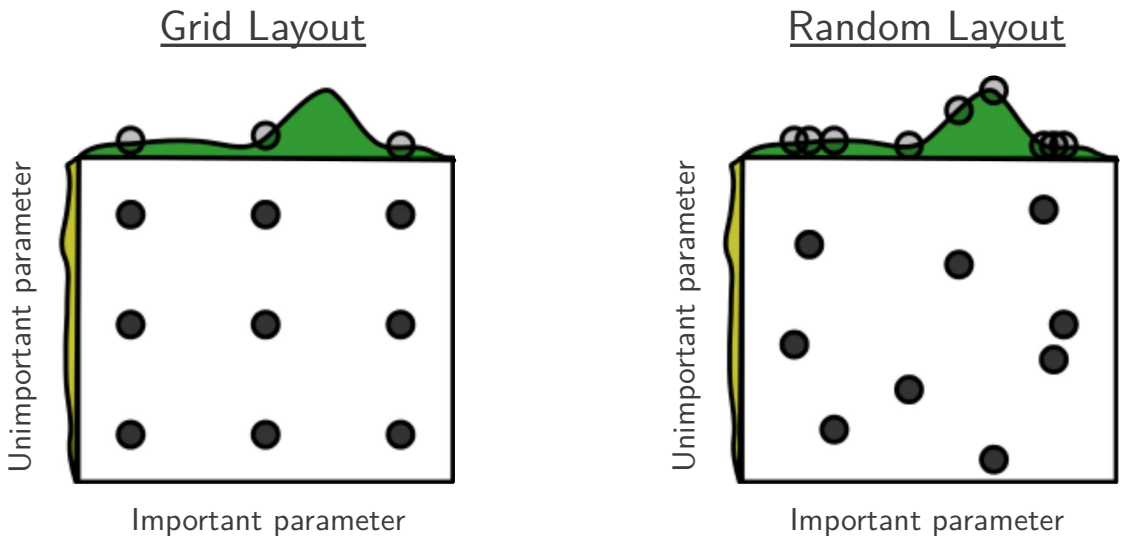
learning rate



learning rate



setting hyperparameters



- compared to grid search, random search allows to explore more values of an important parameter regardless of unimportant parameters
- when the search spans orders of magnitude, draw samples uniformly at random in log space
- start with coarse range and few iterations, gradually move to finer range and more iterations

Bergstra and Bengio. JMLR 2012. Random Search for Hyper-Parameter Optimization.

summary

- stochastic gradient descent and its limitations
- numerical gradient approximation
- analytical computation by decomposing and applying the chain rule
- back-propagation as dynamic programming
- chaining, splitting and sharing
- common patterns between forward and backward flow
- decomposition into unit (forward) and nodes (backward)
- grouping into functions (forward) and blocks (backward)
- learning CIFAR10, validation and hyperparameters