# lecture 6: differentiation

## deep learning for vision

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Inria Rennes-Bretagne Atlantique

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# logistics

- audio of lectures available: link shared via piazza
- related courses including coding assignments linked on course website
- oral presentations: selection of papers by Sunday Dec 16; graduate student to attend presentations on Monday Jan 21
- material marked as XXXX*: some material like examples or details skipped during the lectures is to be studied at home; other material citing recent methods is really optional

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# outline

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

# 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 $f$, we would let this gradient vanish and solve for $\mathbf{x}$

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

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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 $\epsilon$)

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

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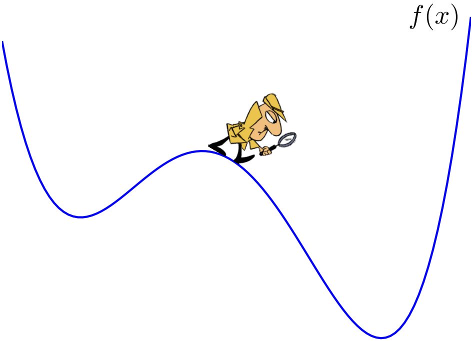
# gradient descent in one dimension




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

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

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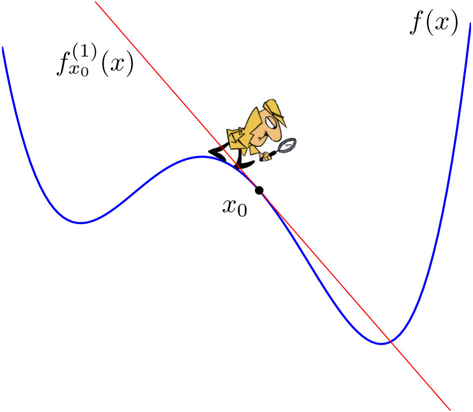


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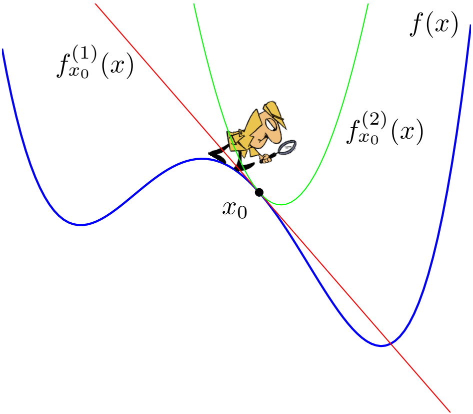


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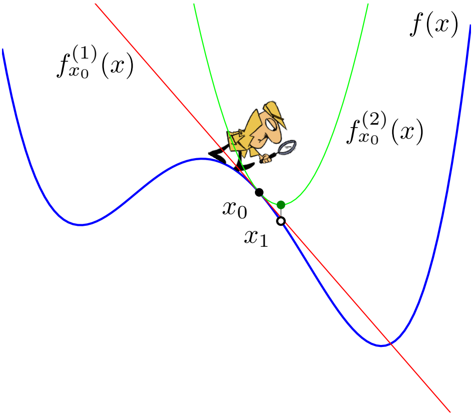


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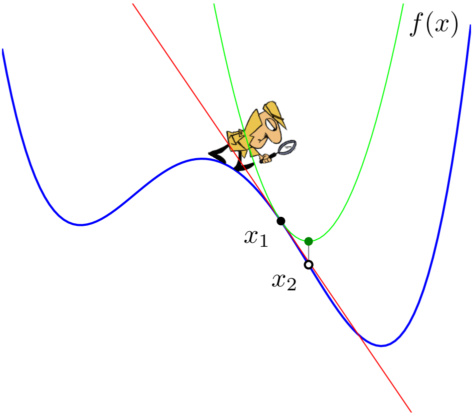


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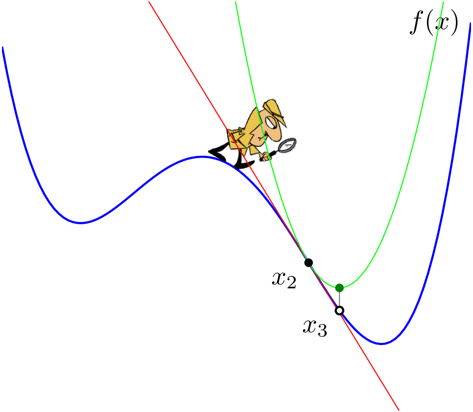


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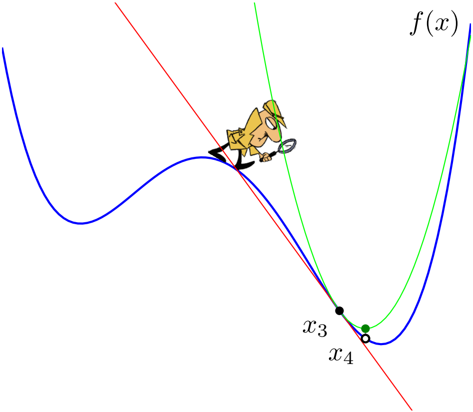


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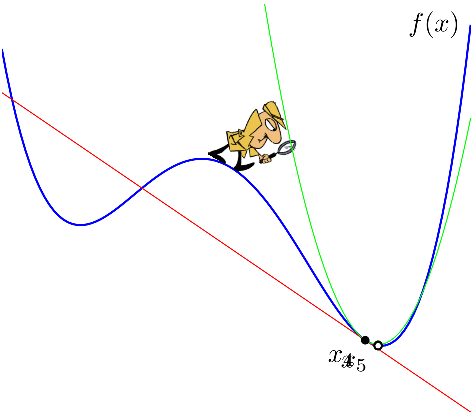


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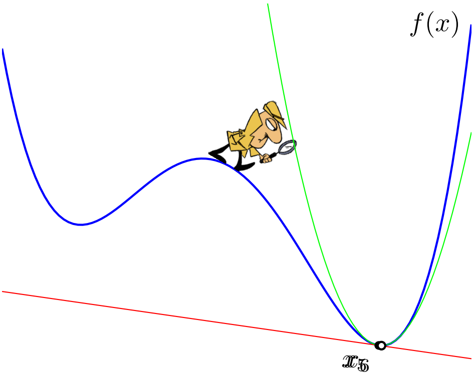


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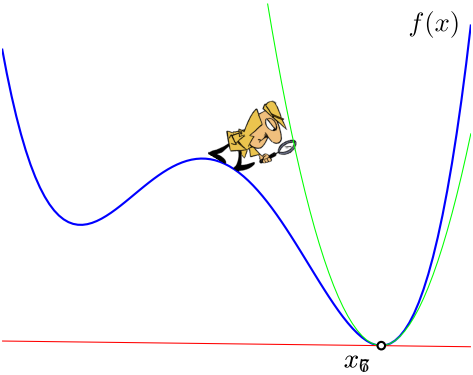


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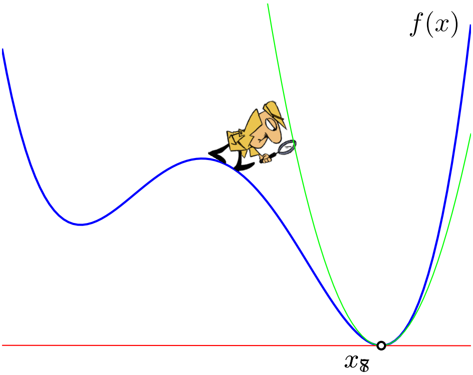


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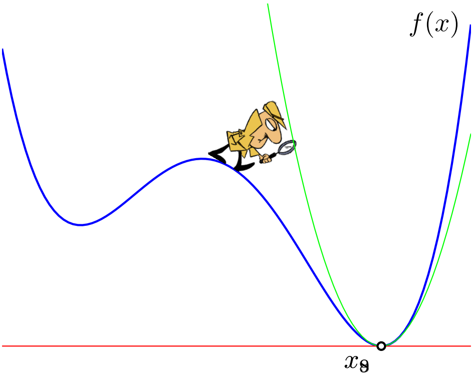


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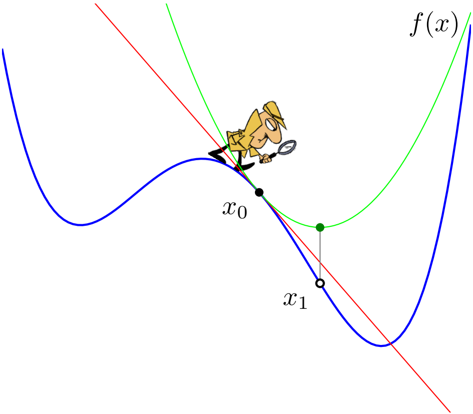


- $\epsilon = 0.14$: $1/\epsilon$ less than actual curvature, does not converge

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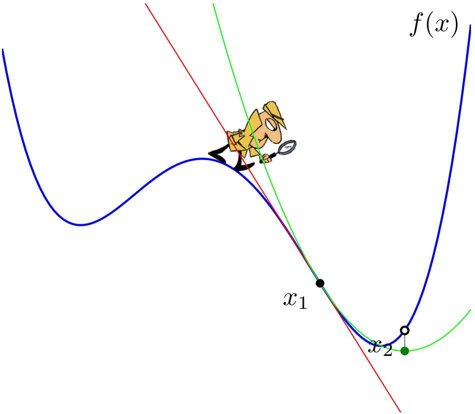


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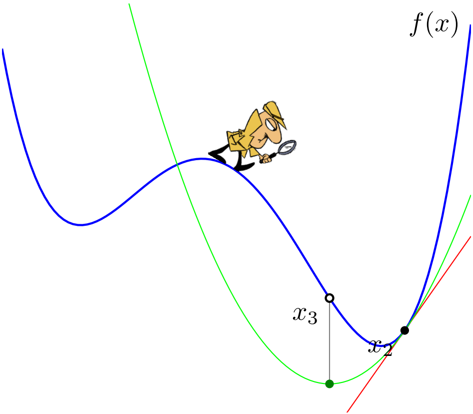


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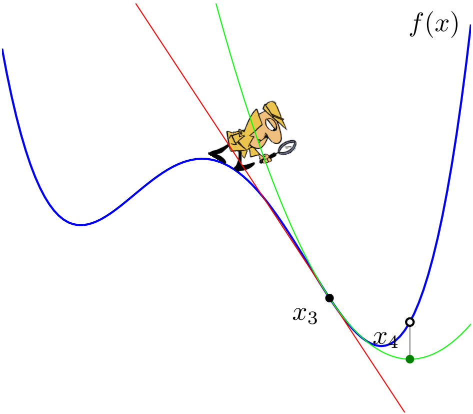


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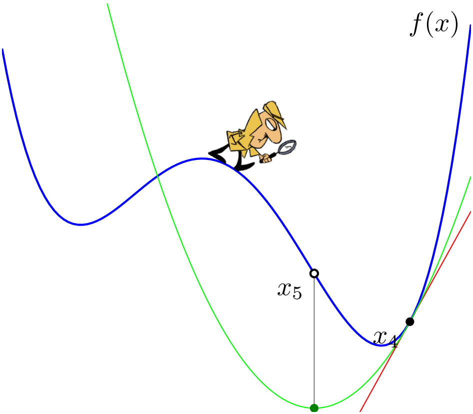


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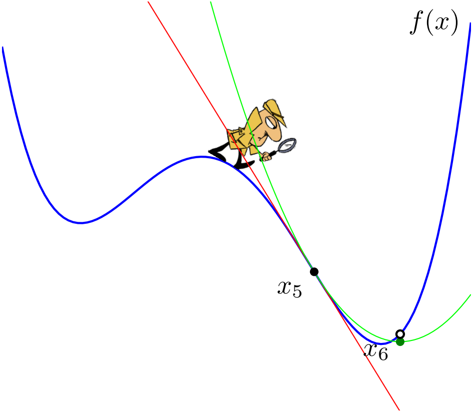


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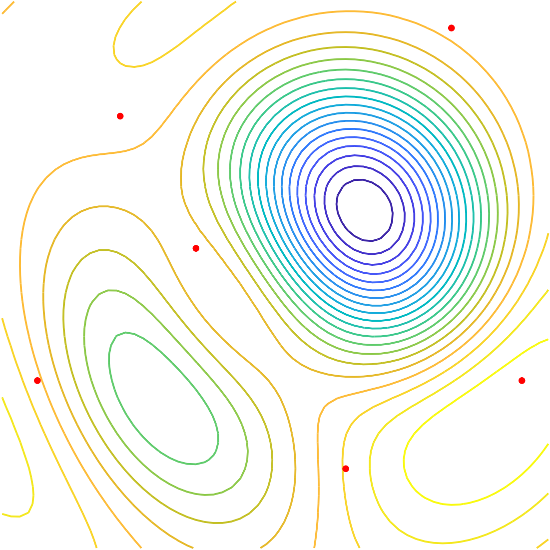
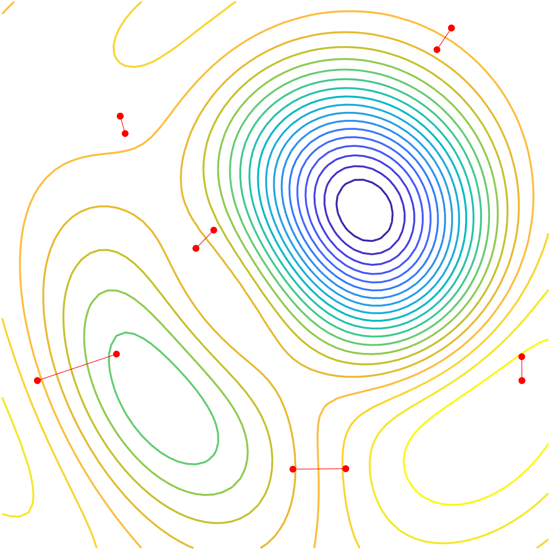
# gradient descent in two dimensions



$\epsilon = 0.14$, iteration $0$

# gradient descent in two dimensions



$\epsilon = 0.14$, iteration 1

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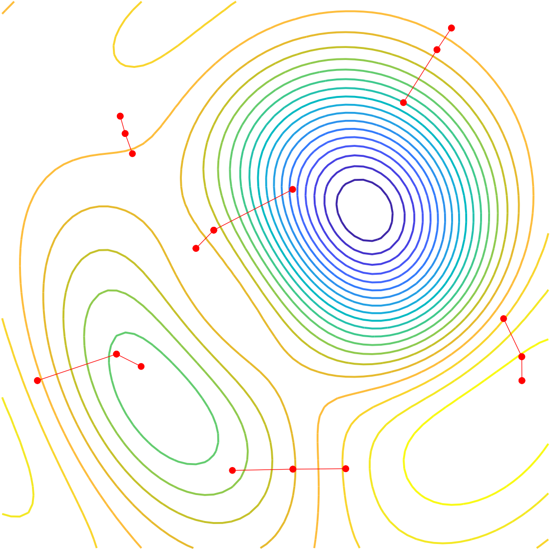
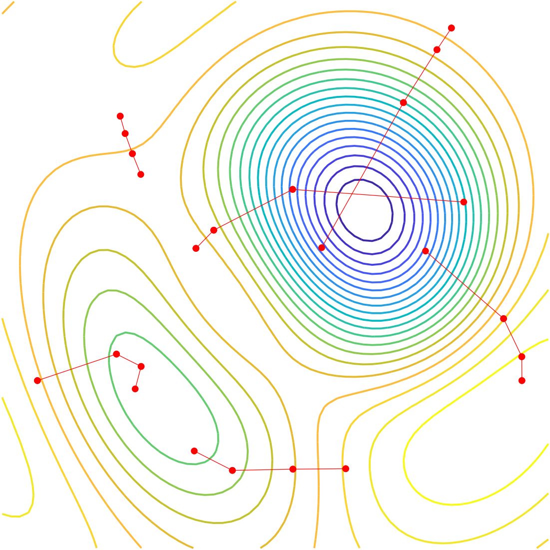


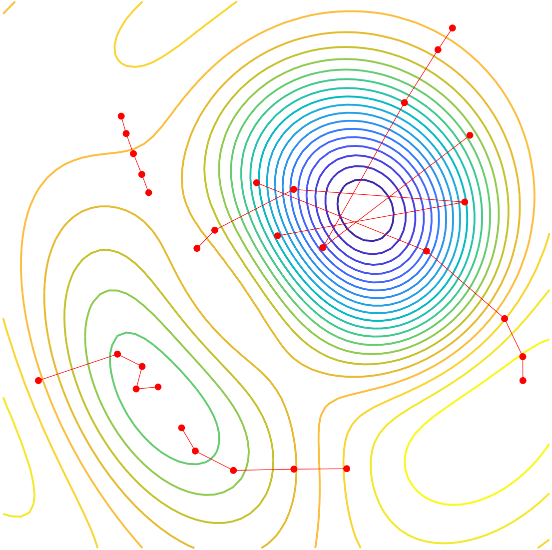
$\epsilon = 0.14$, iteration 2

# gradient descent in two dimensions



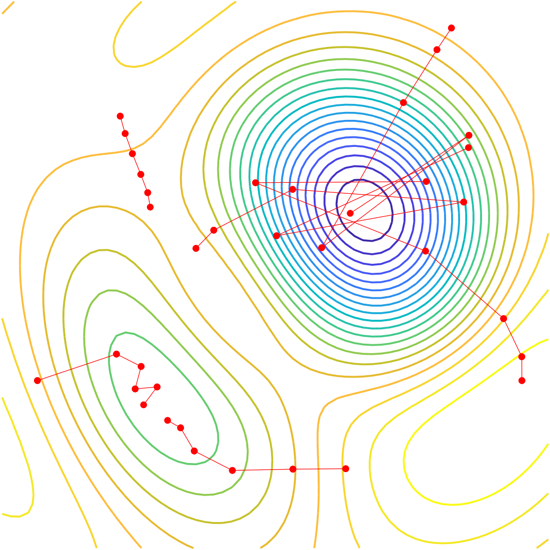
$\epsilon = 0.14$, iteration 3

# gradient descent in two dimensions



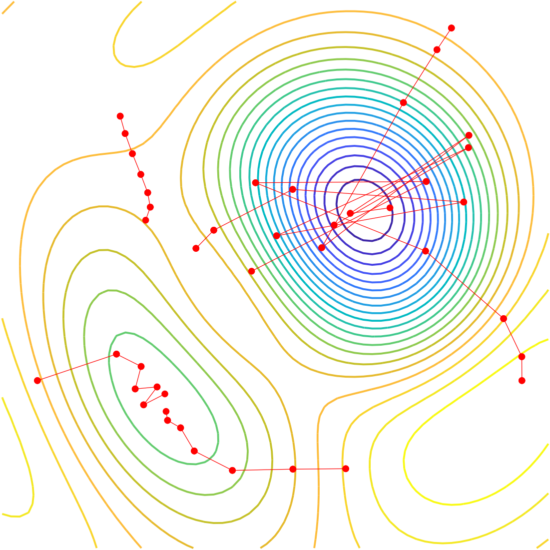
$\epsilon = 0.14$, iteration $4$

# gradient descent in two dimensions



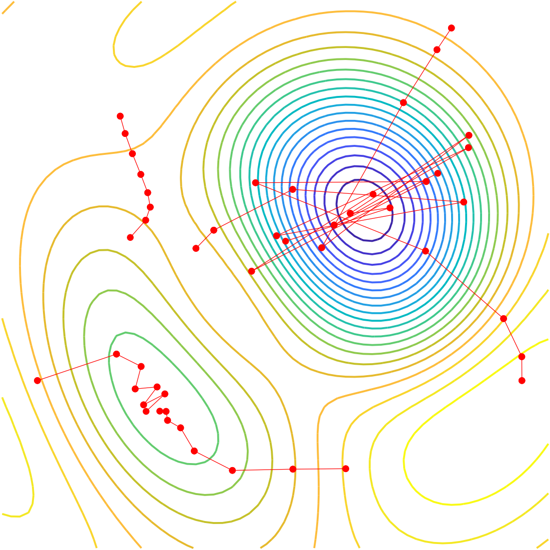
$\epsilon = 0.14$, iteration 5

# gradient descent in two dimensions



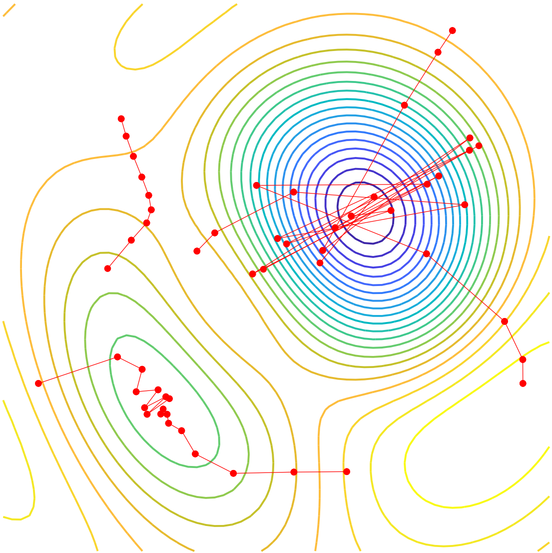
$\epsilon = 0.14$, iteration 6

# gradient descent in two dimensions



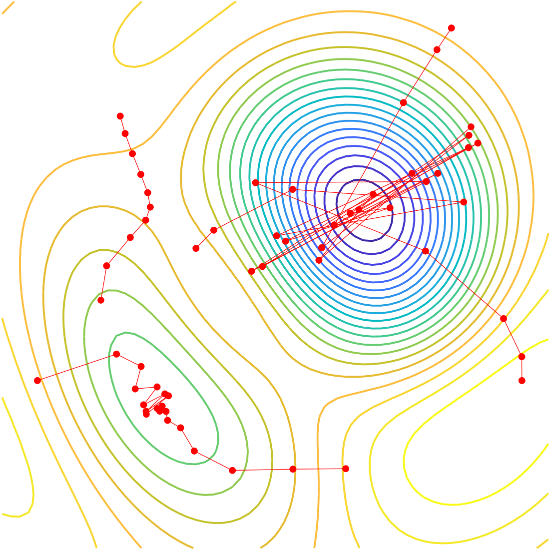
$\epsilon = 0.14$, iteration 7

# gradient descent in two dimensions



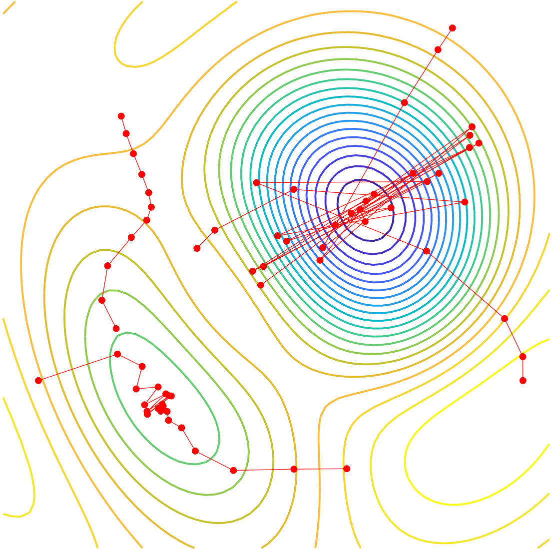
$\epsilon = 0.14$, iteration 8

# gradient descent in two dimensions



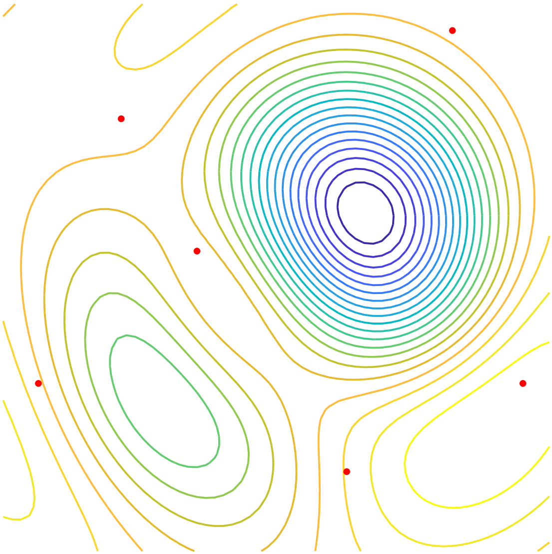
$\epsilon = 0.14$, iteration $9$

# gradient descent in two dimensions



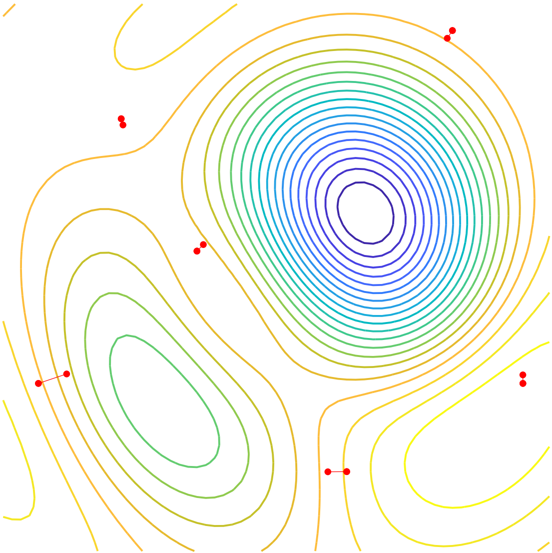
$\epsilon = 0.14$, iteration 10

# gradient descent in two dimensions



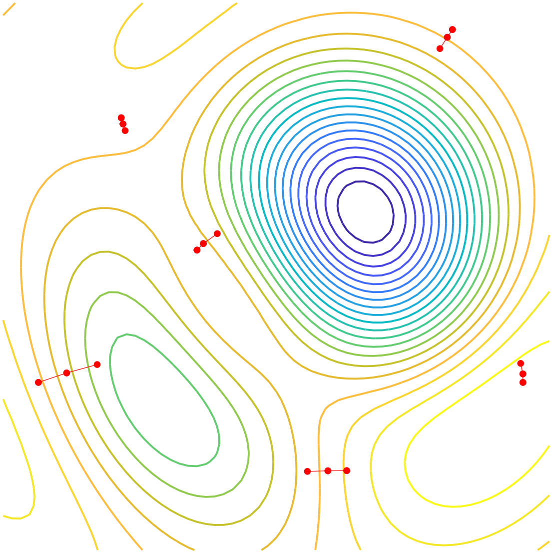
$\epsilon = 0.05$, iteration $0$

# gradient descent in two dimensions



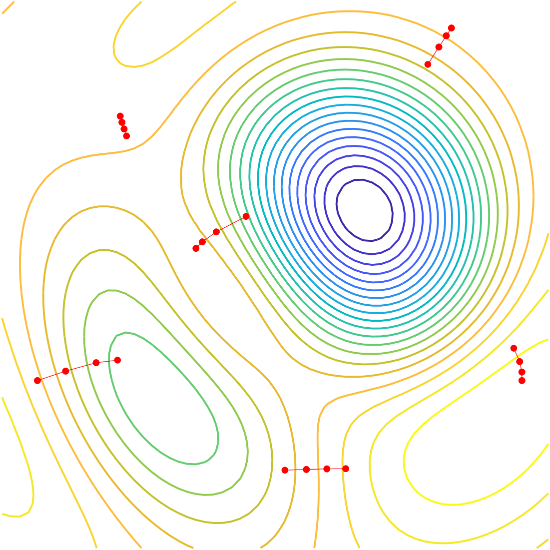
$\epsilon = 0.05$, iteration 1

# gradient descent in two dimensions



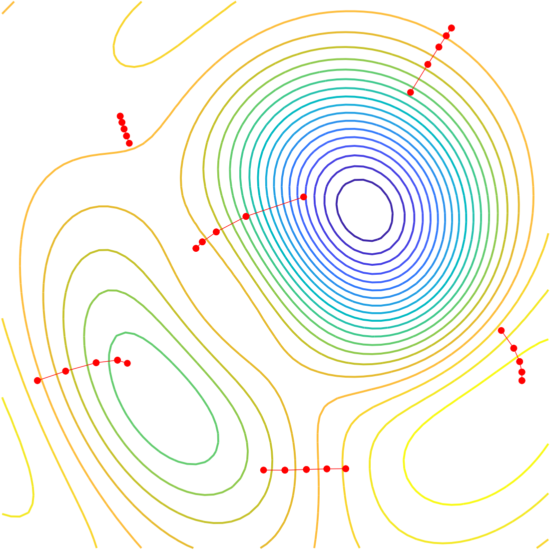
$\epsilon = 0.05$, iteration 2

# gradient descent in two dimensions



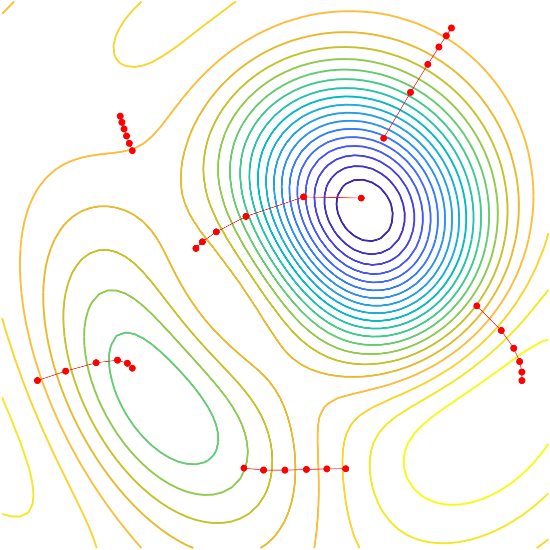
$\epsilon = 0.05$, iteration 3

# gradient descent in two dimensions



$\epsilon = 0.05$, iteration 4

# gradient descent in two dimensions



$\epsilon = 0.05$, iteration 5

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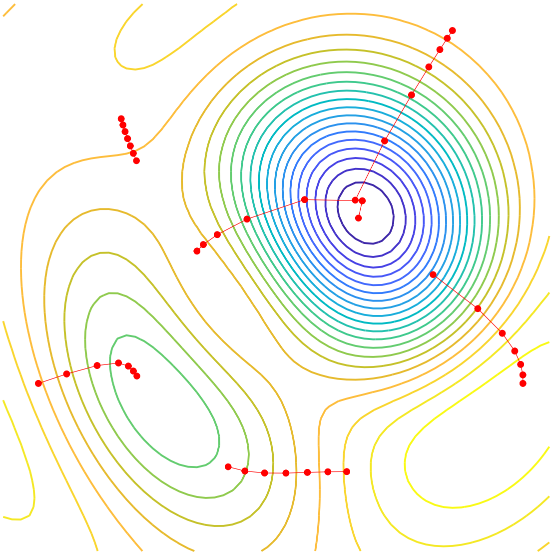
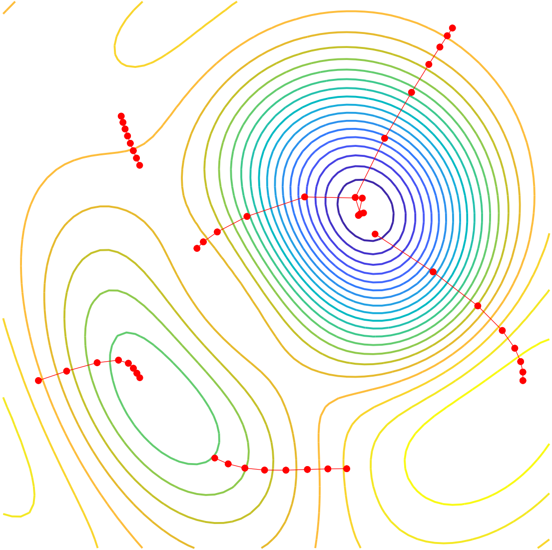


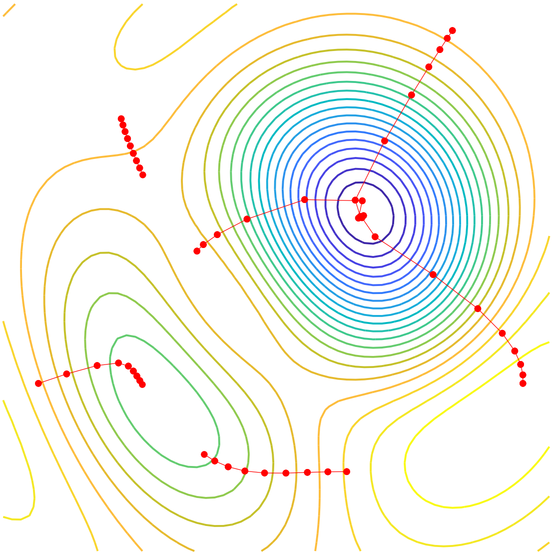
$\epsilon = 0.05$, iteration 6

# gradient descent in two dimensions



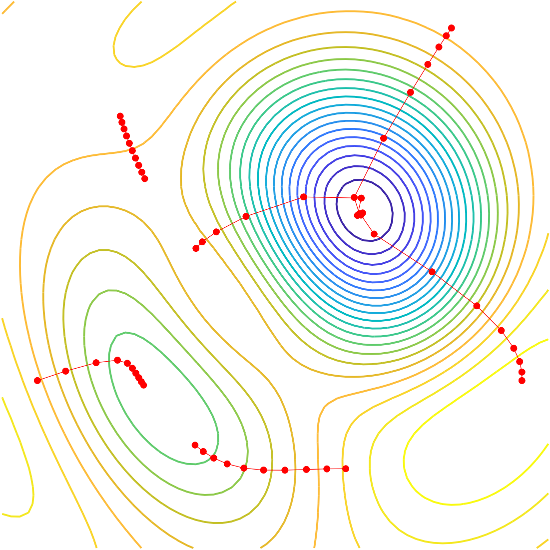
$\epsilon = 0.05$, iteration 7

# gradient descent in two dimensions



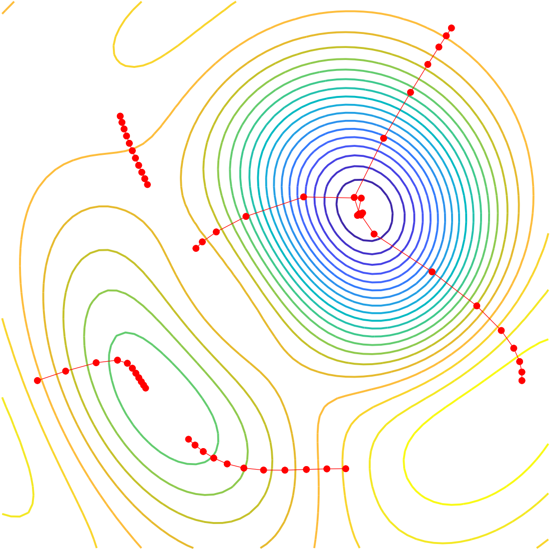
$\epsilon = 0.05$, iteration $8$

# gradient descent in two dimensions



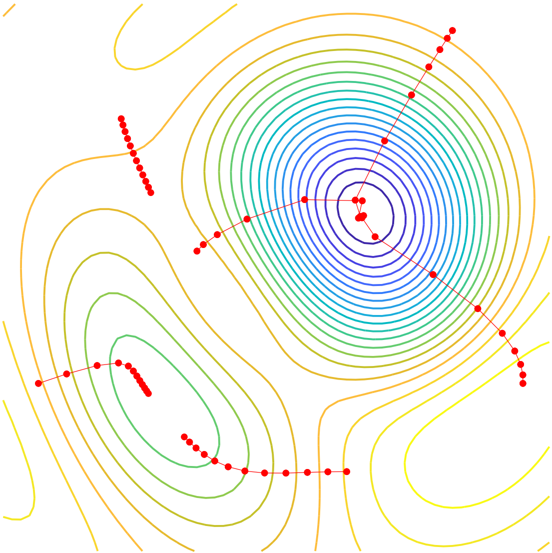
$\epsilon = 0.05$, iteration 9

# gradient descent in two dimensions



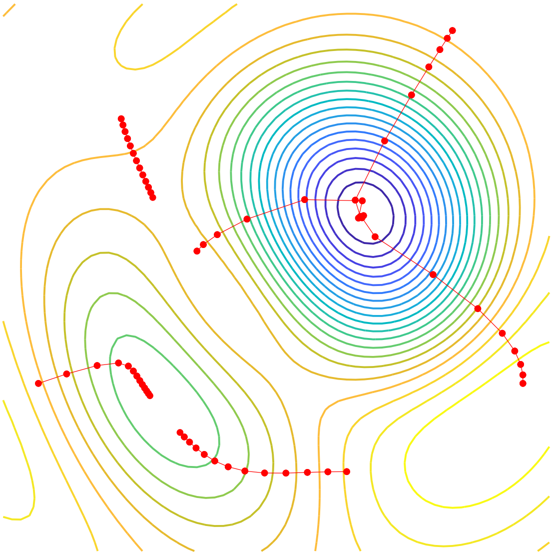
$\epsilon = 0.05$, iteration 10

# gradient descent in two dimensions



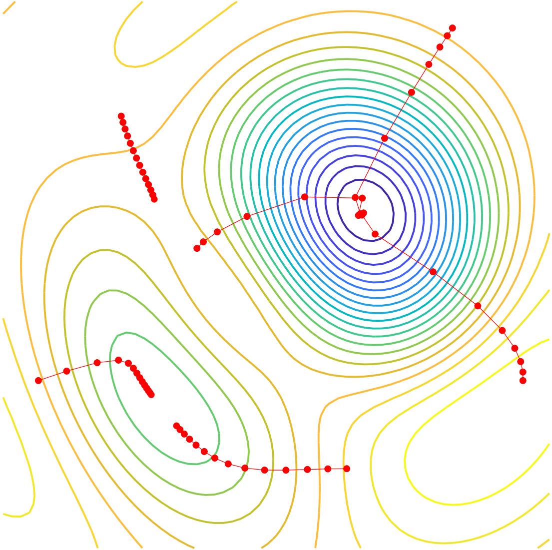
$\epsilon = 0.05$, iteration 11

# gradient descent in two dimensions



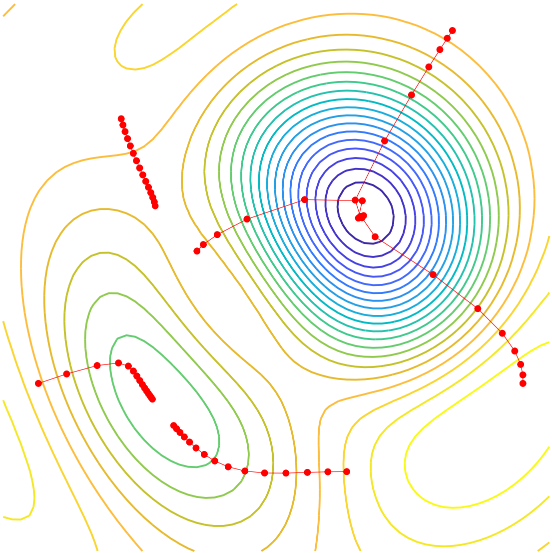
$\epsilon = 0.05$, iteration 12

# gradient descent in two dimensions



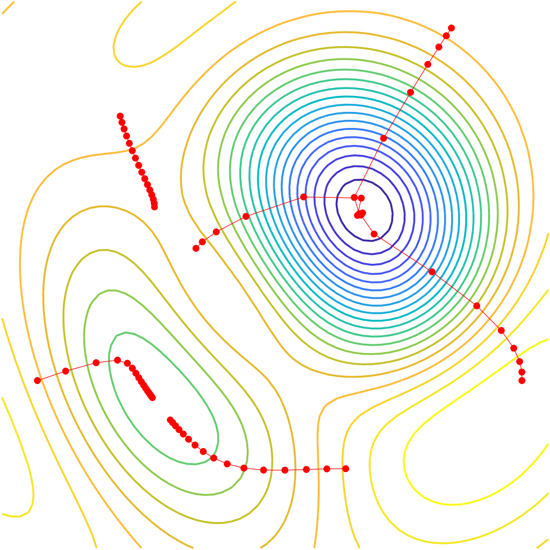
$\epsilon = 0.05$, iteration 13

# gradient descent in two dimensions



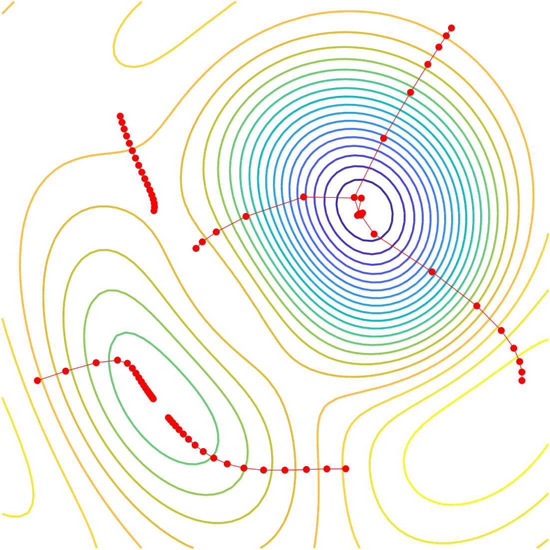
$\epsilon = 0.05$, iteration 14

# gradient descent in two dimensions



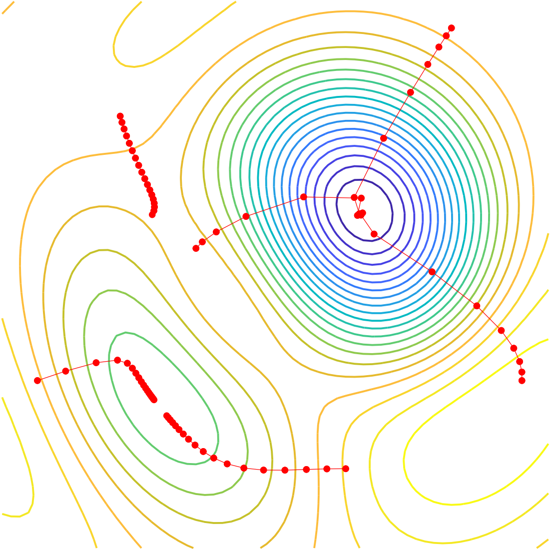
$\epsilon = 0.05$, iteration 15

# gradient descent in two dimensions



$\epsilon = 0.05$, iteration 16

# gradient descent in two dimensions



$\epsilon = 0.05$, iteration 17

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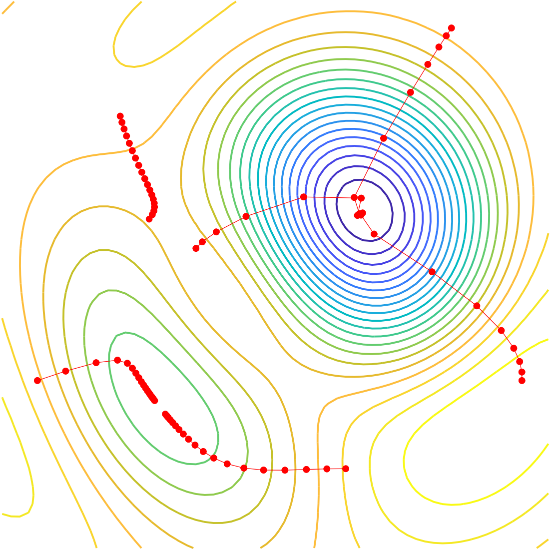
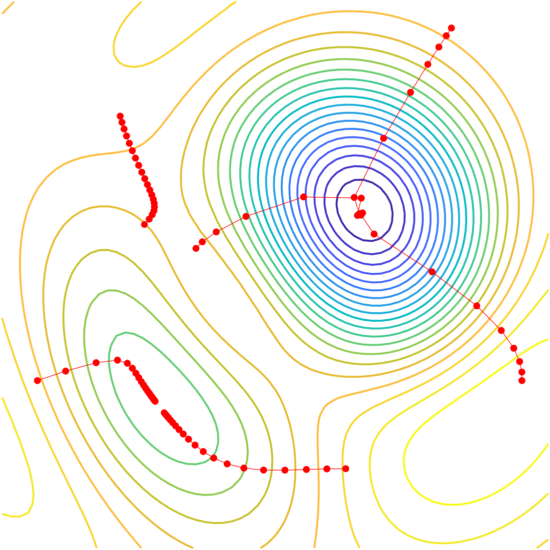


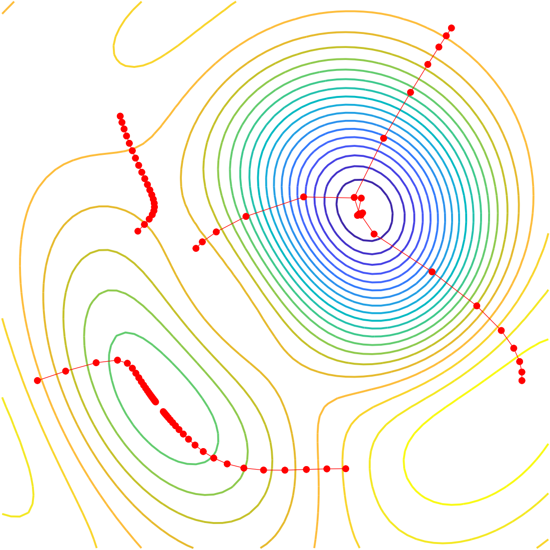
$\epsilon = 0.05$, iteration 18

# gradient descent in two dimensions



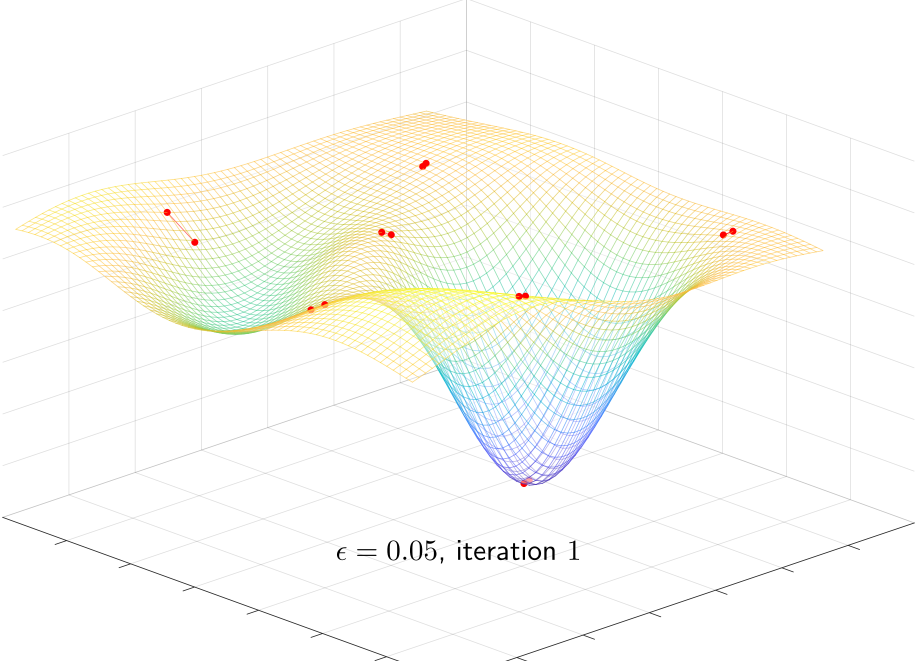
$\epsilon = 0.05$, iteration 19

# gradient descent in two dimensions



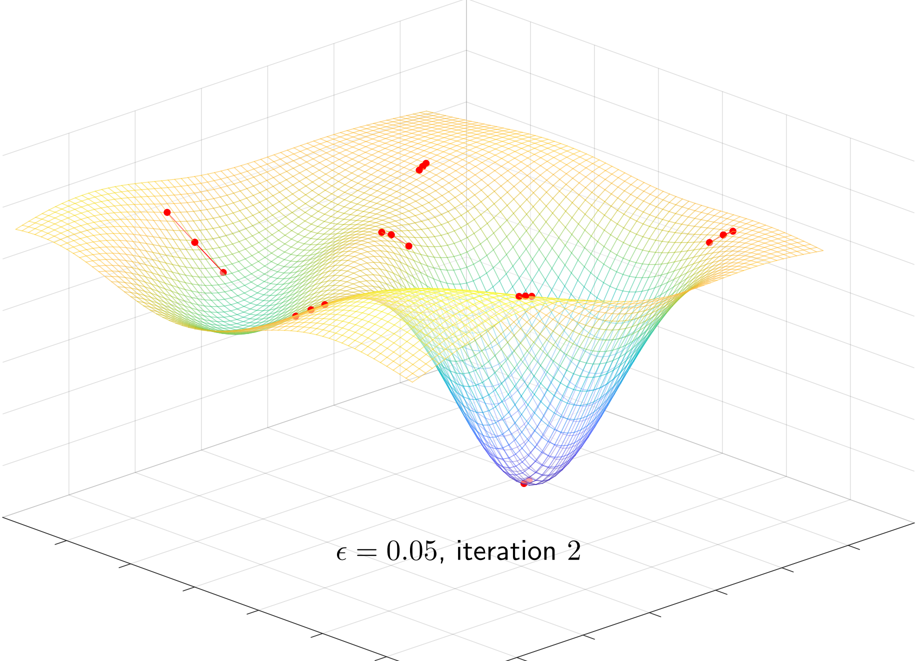
$\epsilon = 0.05$, iteration 20

# gradient descent in two dimensions



$\epsilon = 0.05$, iteration 1

# gradient descent in two dimensions



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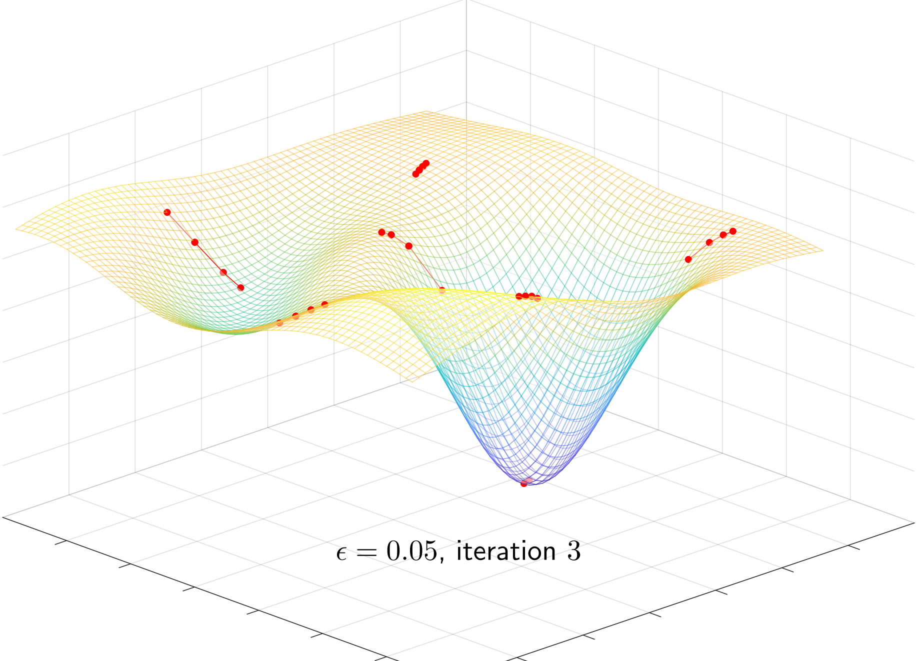

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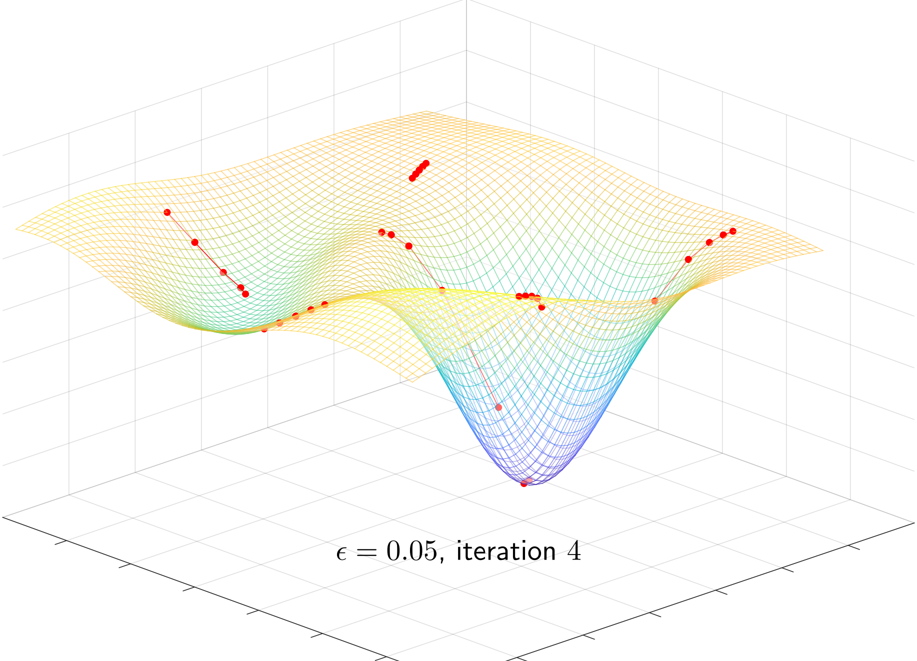

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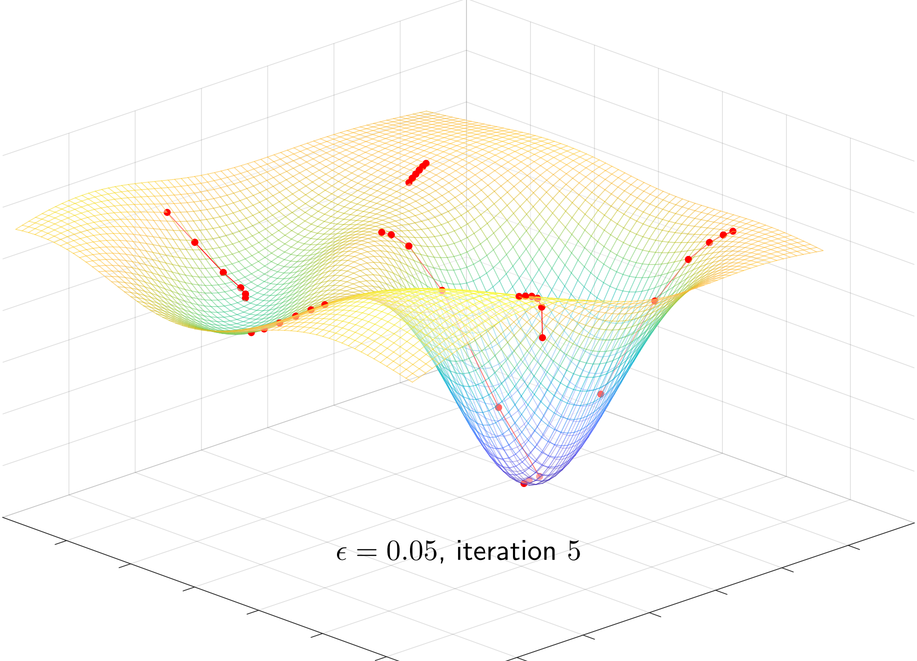
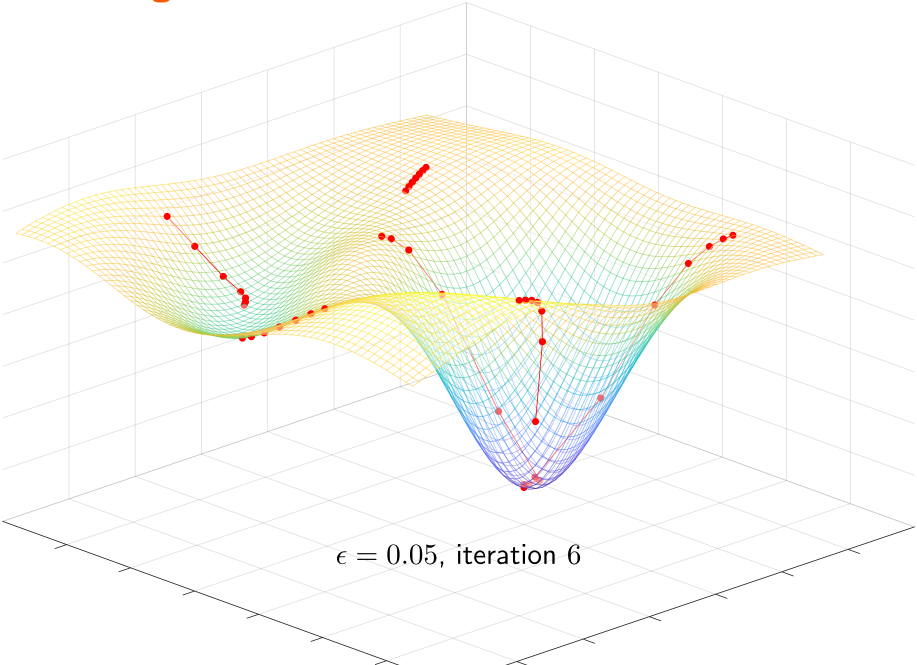


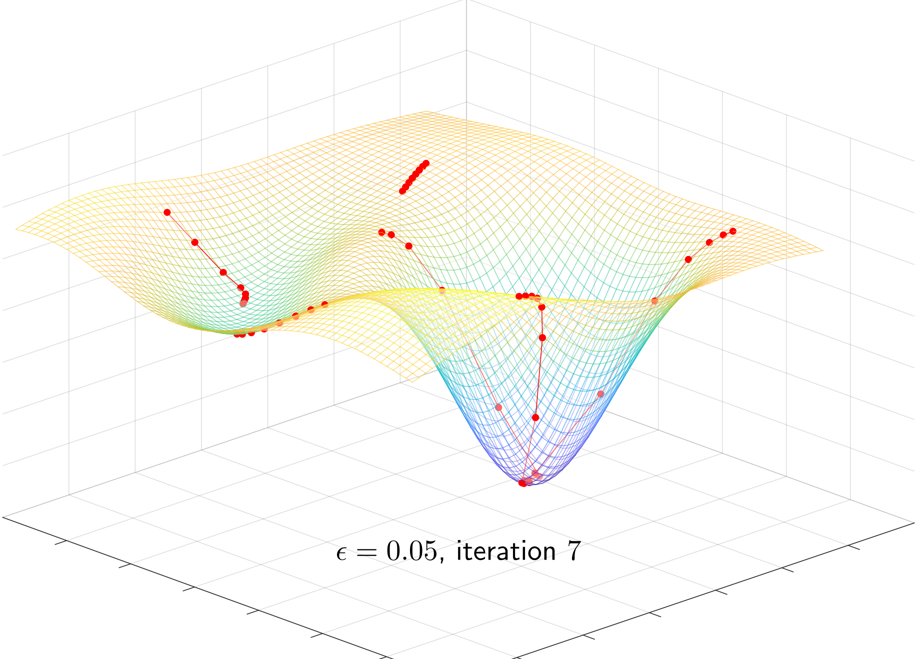
$\epsilon = 0.05$, iteration 5

# gradient descent in two dimensions



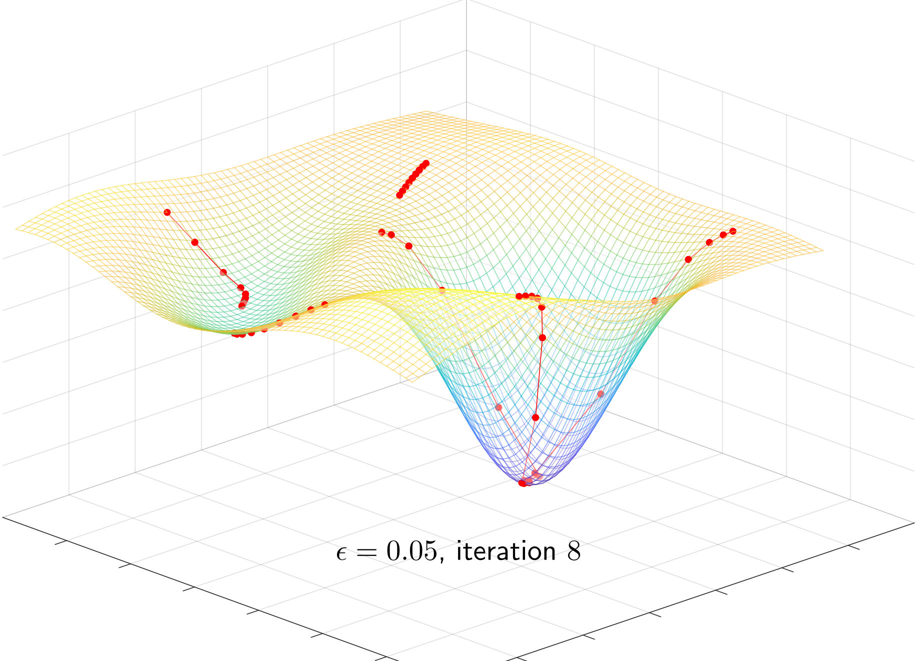
$\epsilon = 0.05$, iteration 6

# gradient descent in two dimensions



$\epsilon = 0.05$, iteration 7

# gradient descent in two dimensions



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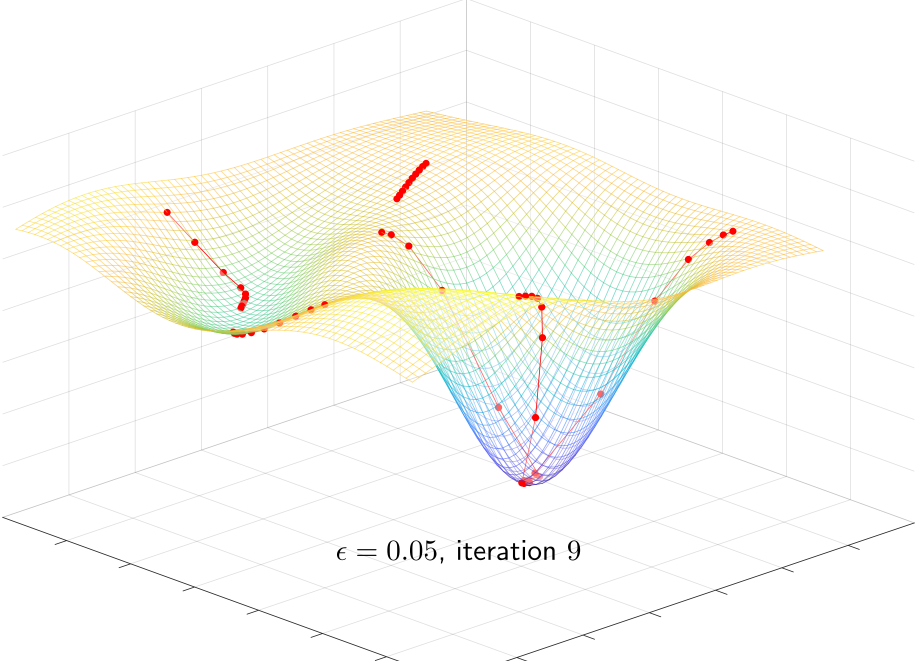
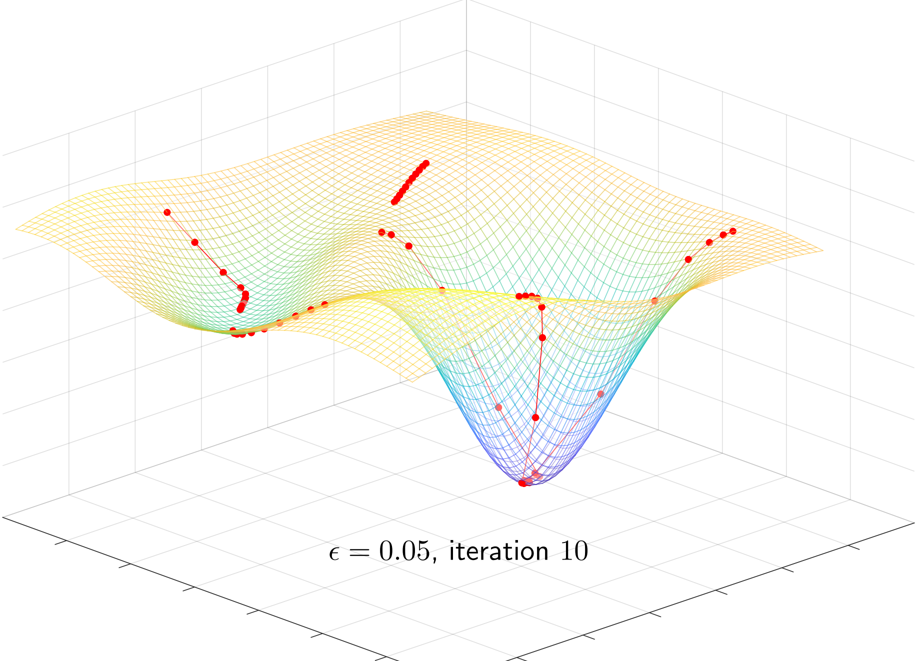


$\epsilon = 0.05$, iteration 9

# gradient descent in two dimensions



$\epsilon = 0.05$, iteration 10

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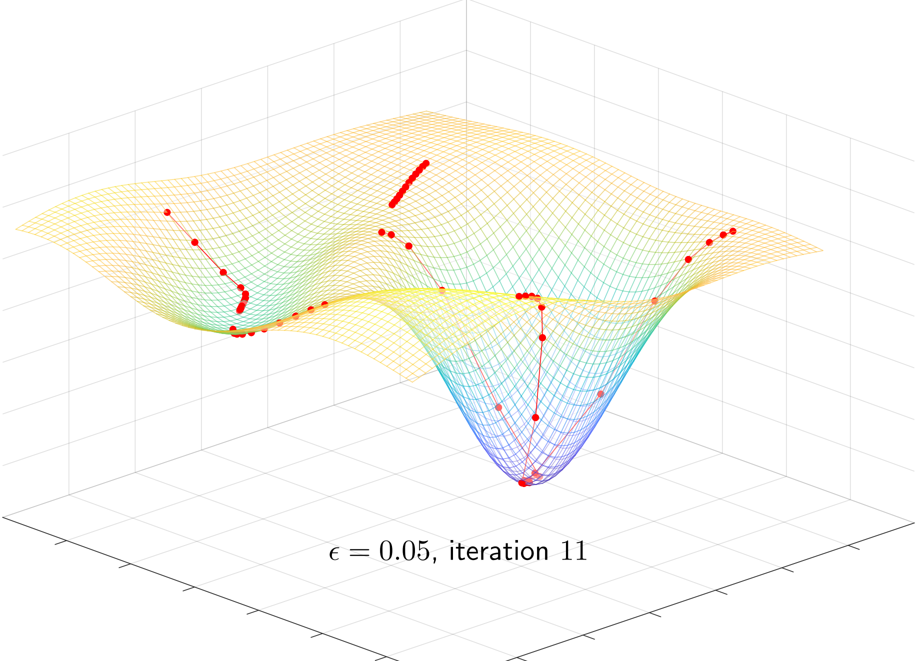

$\epsilon = 0.05$, iteration 11

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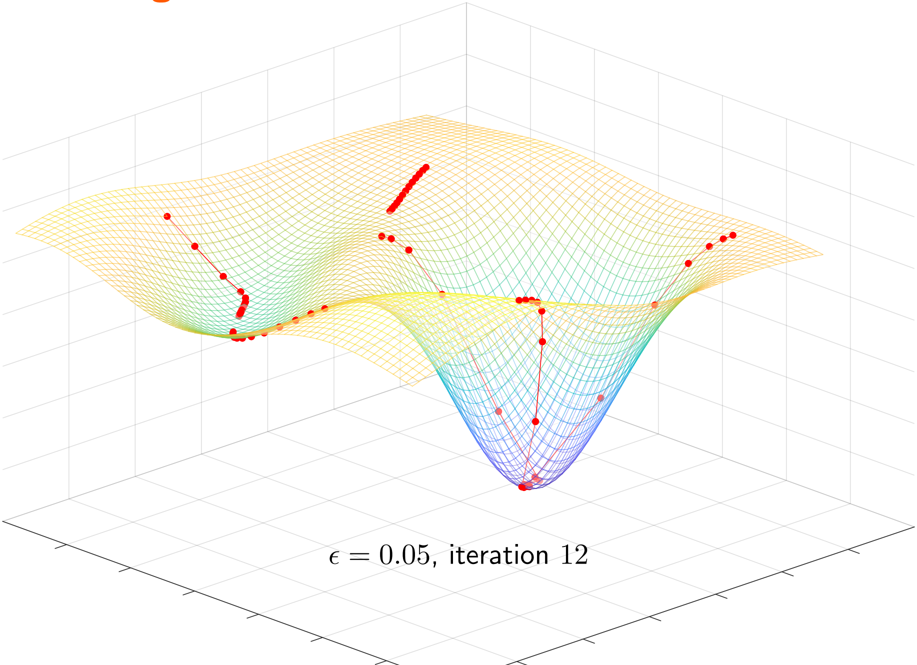

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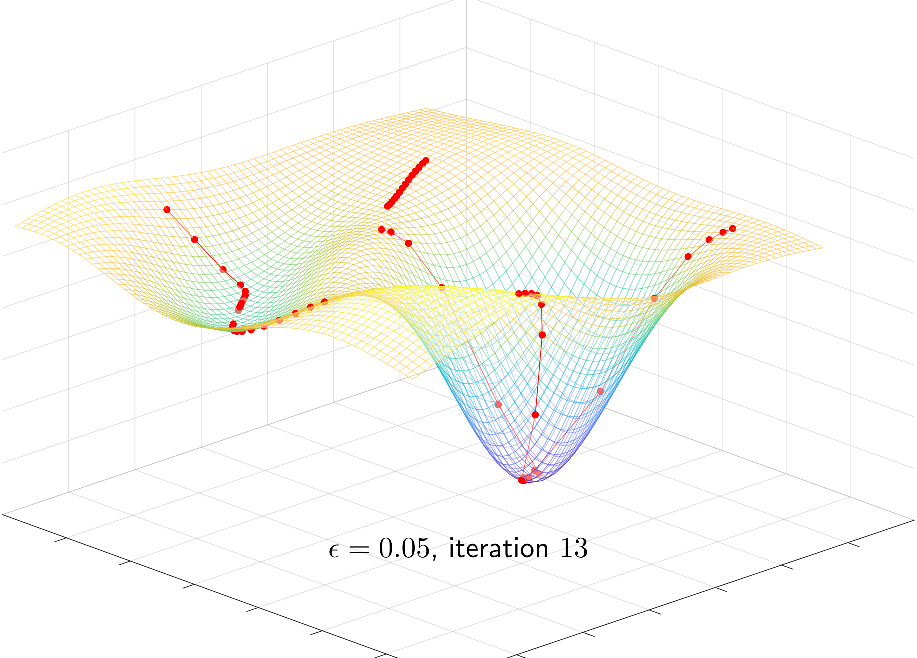
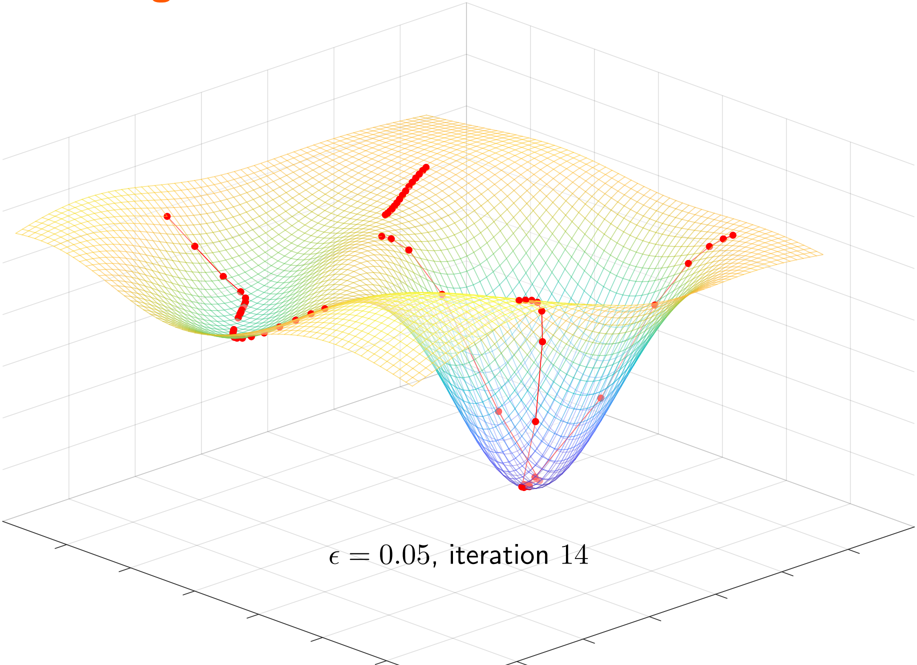


$\epsilon = 0.05$, iteration 13

# gradient descent in two dimensions



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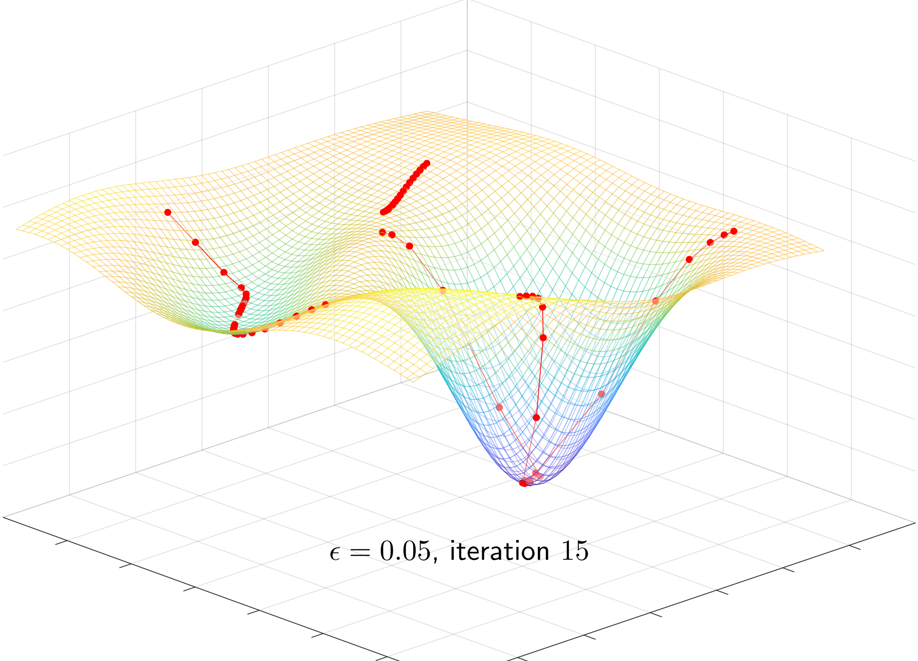

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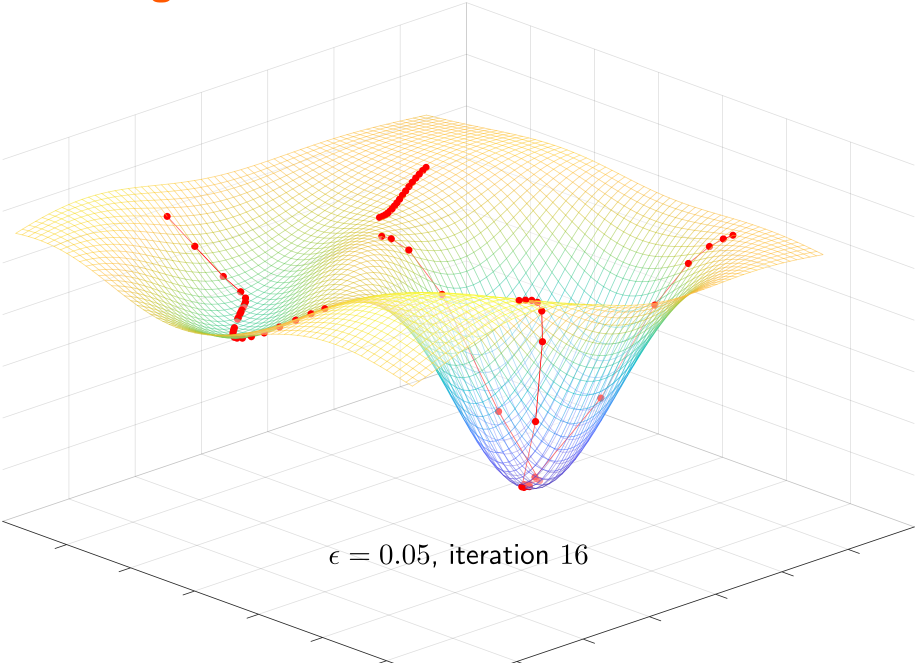

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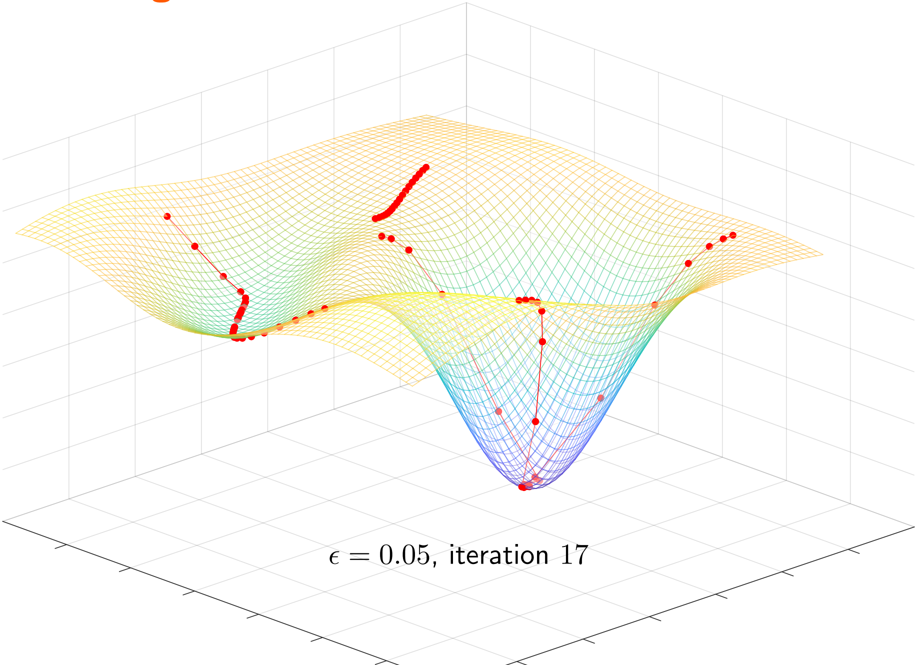

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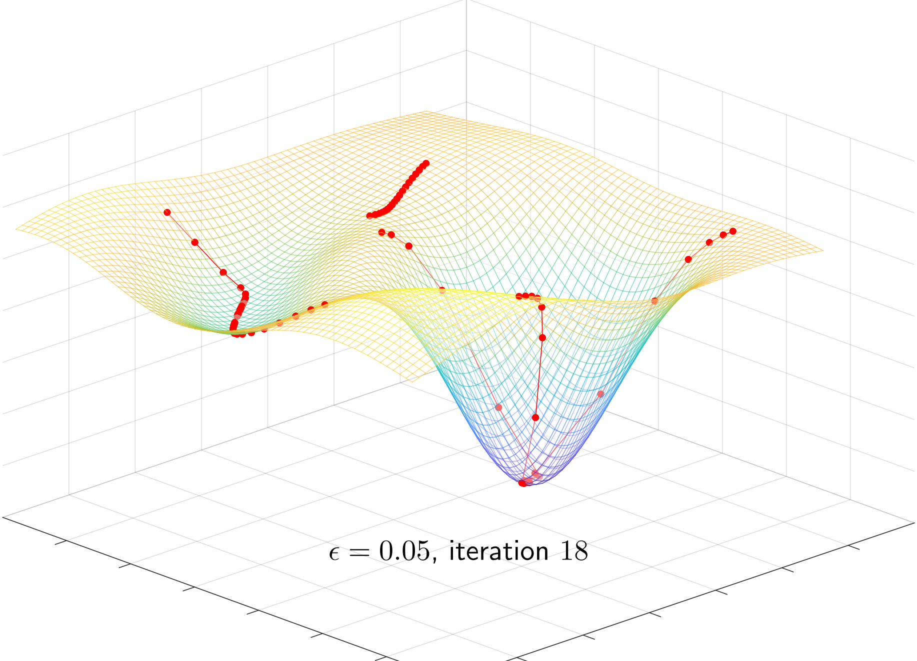

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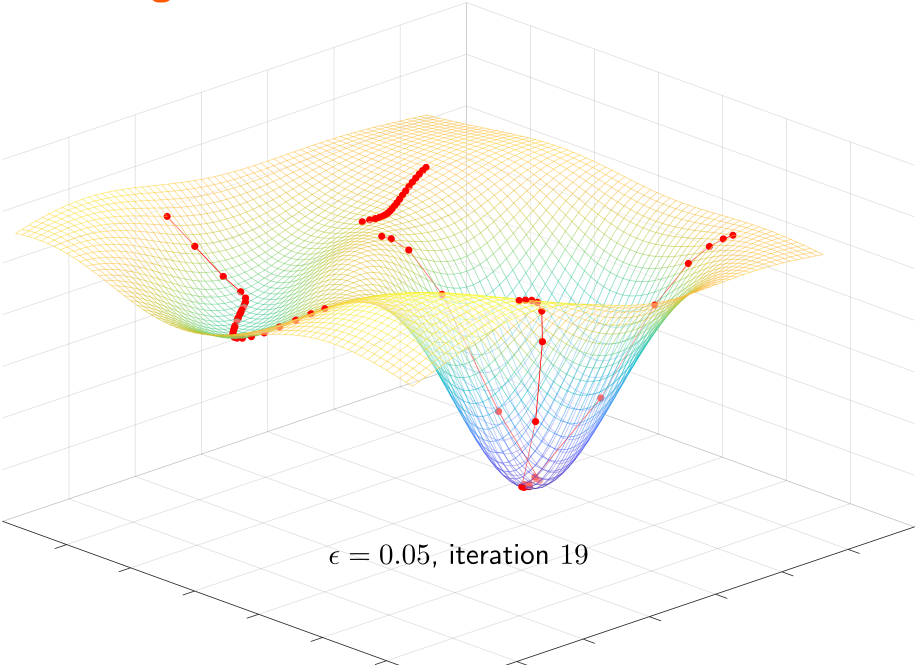

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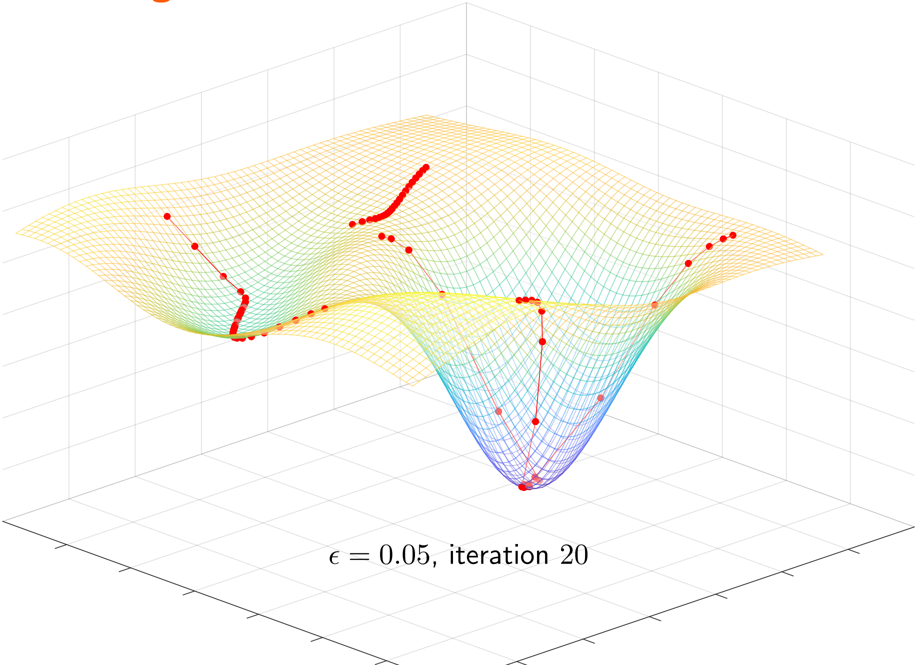

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# problems

- $f$ 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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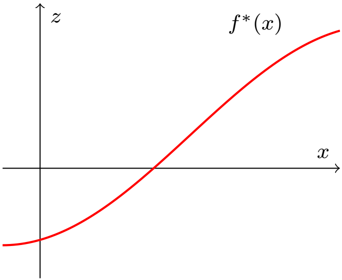
# sequential estimation

[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.

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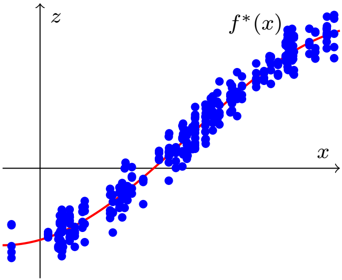


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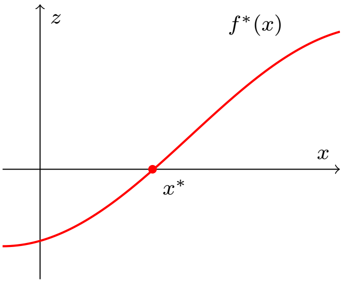


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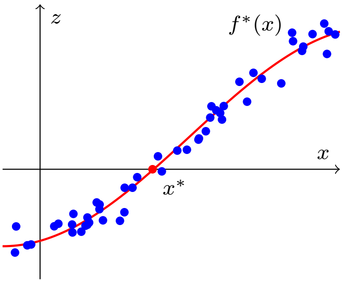


- then we can estimate $x^*$ sequentially

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

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 $\nabla E$, 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

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

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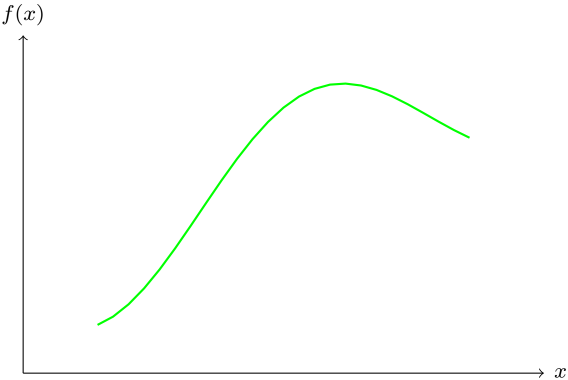
# gradient computation

# numerical approximation



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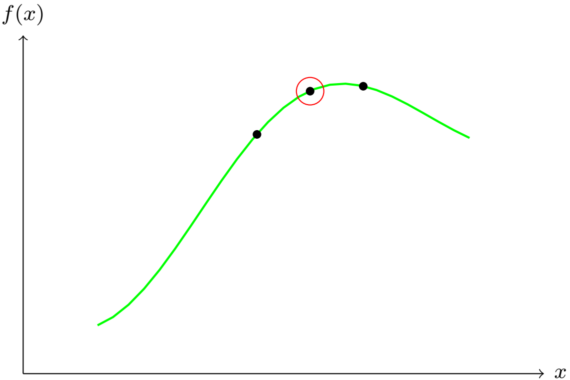

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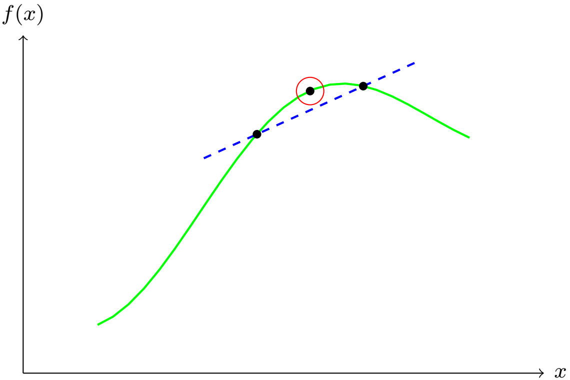

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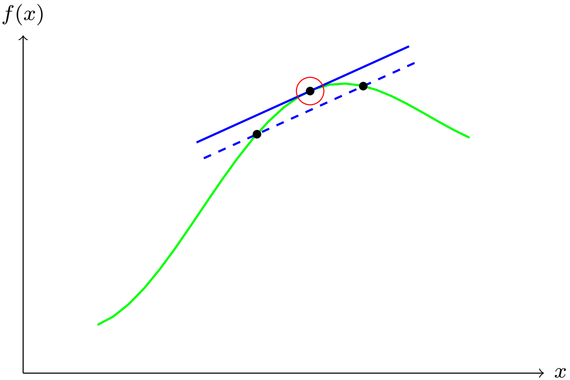


$$\frac{df}{dx}(x) \approx \frac{f(x+\delta) - f(x-\delta)}{2\delta}$$

# numerical approximation

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

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

- each partial derivative $\frac{\partial f}{\partial x_i}$ can be approximated at $\mathbf{x}$ by the 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 $\mathbf{e}_i$ is the $i$ standard basis vector of $\mathbb{R}^m$

- in practice, the smallest $\delta$ 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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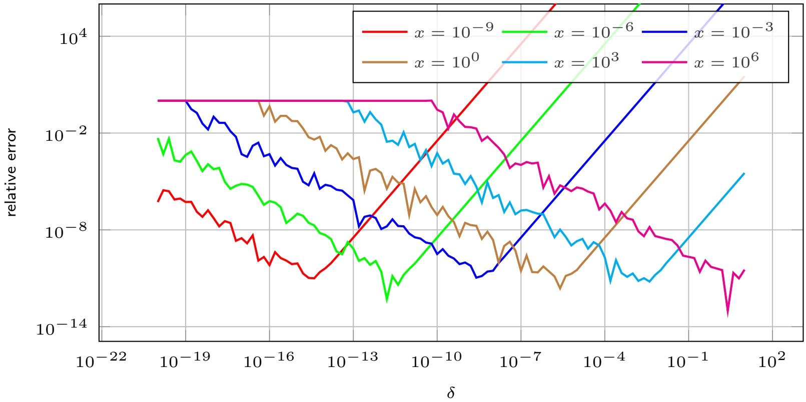
# example




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

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

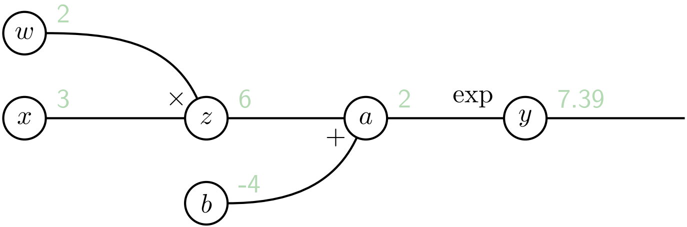
# numerical vs. analytical

- apart from accuracy issues, the numerical approximation is impractical in high dimensions: one evaluation of $\Delta f$ 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




- $y = e^{wx+b}$ is broken down into $y = e^a$, $a = z + b$, $z = wx$
- we seek $\frac{\partial y}{\partial w}$, $\frac{\partial y}{\partial x}$, $\frac{\partial y}{\partial b}$ for $(w, x, b) = (2, 3, -4)$
- $\frac{\partial y}{\partial y} = 1$, $\frac{\partial y}{\partial a} = e^a = 7.39$, $\frac{\partial y}{\partial b} = \frac{\partial y}{\partial a}\frac{\partial a}{\partial b} = \frac{\partial y}{\partial a} = 7.39$,
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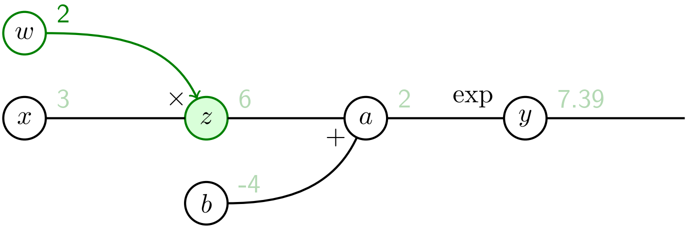


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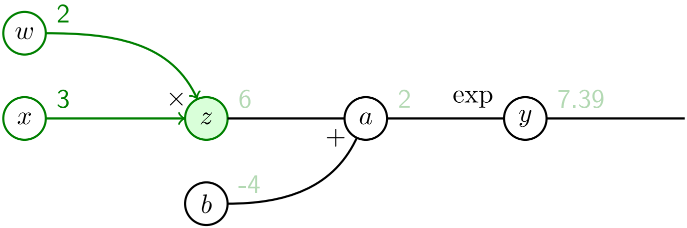


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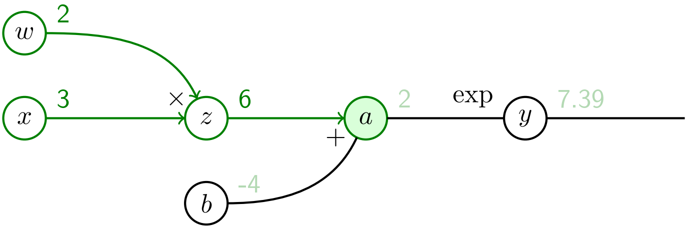


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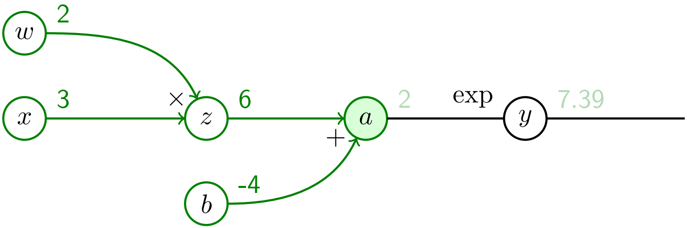


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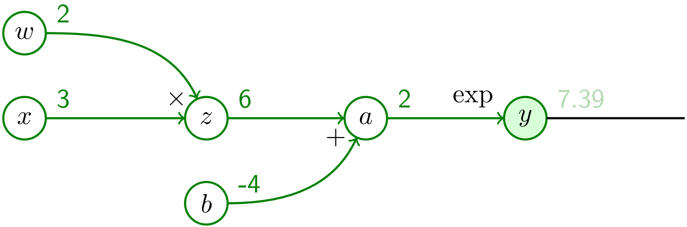


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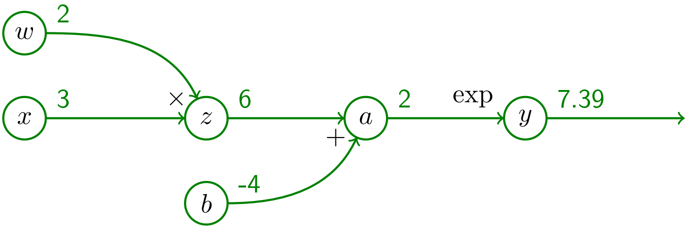


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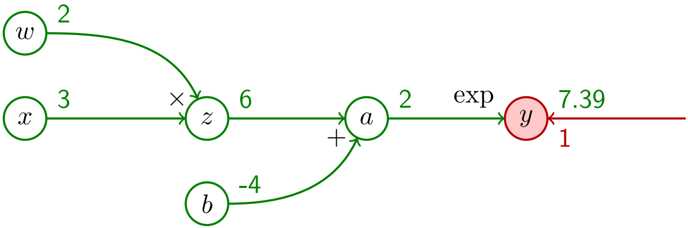


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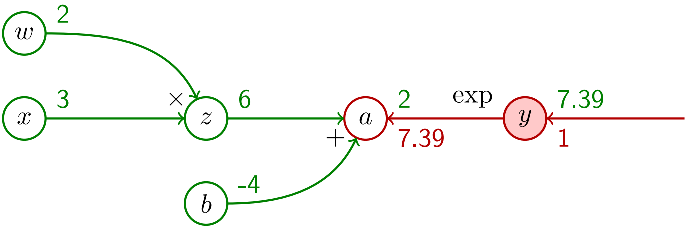


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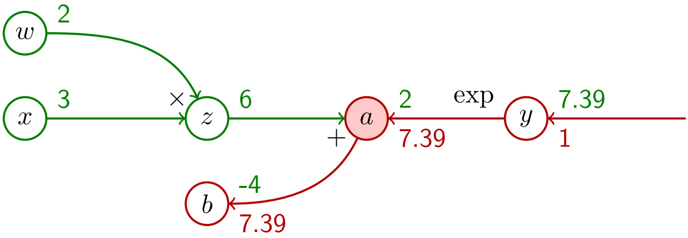


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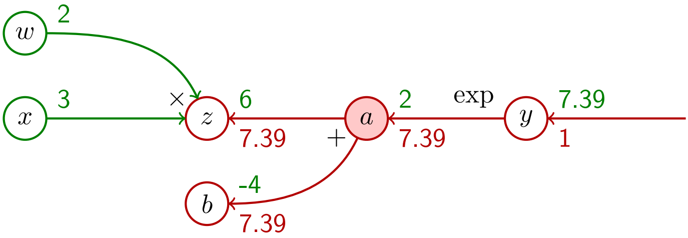


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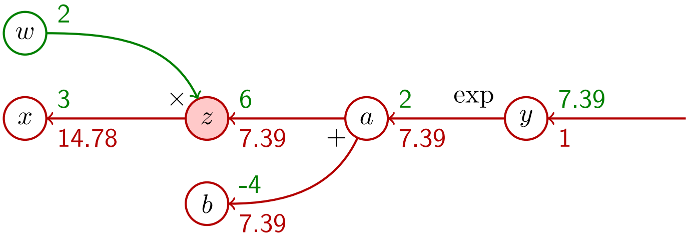


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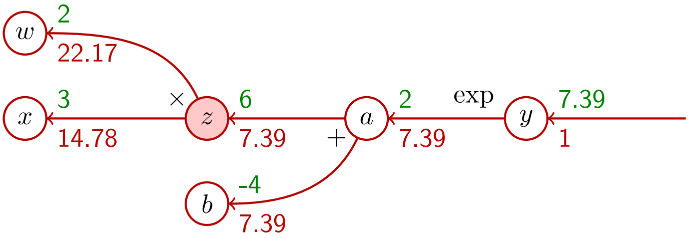


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# vector functions: derivative

- a function $f : \mathbb{R}^p \to \mathbb{R}^q$ is differentiable at $\mathbf{x}$ if there is a $q \times p$ matrix $A$ such that

$$\frac{f(\mathbf{x}+\mathbf{h}) - f(\mathbf{x}) - A \cdot \mathbf{h}}{|\mathbf{h}|} \to \mathbf{0}$$

  as $\mathbf{h} \to \mathbf{0}$; matrix $A$ is the derivative of $f$ at $\mathbf{x}$, denoted as $Df(\mathbf{x})$

- if

$$f(\mathbf{x}) = A\mathbf{x}$$

  then

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# vector functions: derivative vs. Jacobian

- given $f = (f_1, \dots, f_q) : \mathbb{R}^p \to \mathbb{R}^q$ whose its partial derivatives exist at $\mathbf{x}$, and $\mathbf{y} = f(\mathbf{x})$, its Jacobian matrix at $\mathbf{x}$ can be written as

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

- if $f$ is differentiable at $\mathbf{x}$, its derivative at $\mathbf{x}$ is

$$Df(\mathbf{x}) := \begin{pmatrix} D_1 f_1 & \dots & D_p f_1 \\ \vdots & \ddots & \vdots \\ D_1 f_q & \dots & D_p f_q \end{pmatrix} (\mathbf{x})$$

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# scalar functions: derivative vs. gradient

- the gradient of a scalar $f : \mathbb{R}^p \to \mathbb{R}$ with respect to an input vector $\mathbf{x}$ is a column vector in $\mathbb{R}^p$, the same size as $\mathbf{x}$

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

- in contrast, the derivative is an $1 \times p$ row vector

$$Df(\mathbf{x}) := \begin{pmatrix} \frac{\partial f}{\partial x_1} & \ldots & \frac{\partial f}{\partial x_p} \end{pmatrix} = (\nabla f)^\top$$

- the following analysis uses derivatives/Jacobians, so we will transpose them to make them compatible with $\mathbf{x}$

# 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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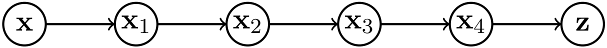

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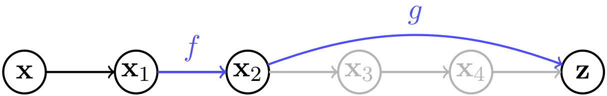

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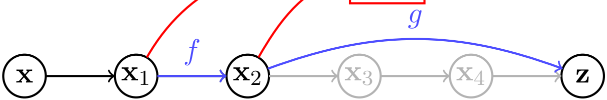

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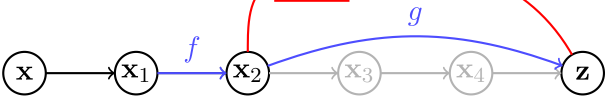

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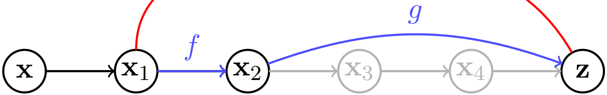

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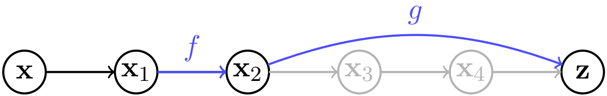


- now, for all $i$, let us call the partial derivatives

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

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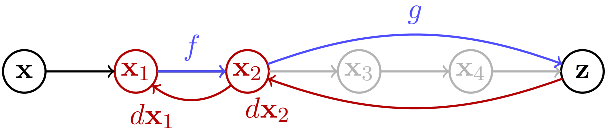
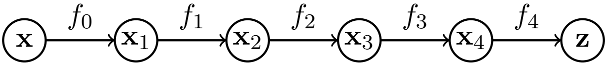



- then, we are back-propagating from $d\mathbf{x}_2$ to $d\mathbf{x}_1$

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

# 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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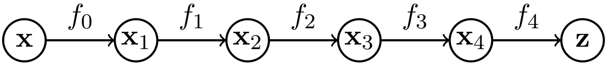


- we apply the chain rule

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

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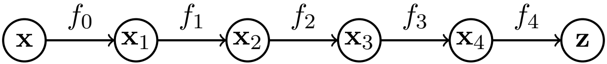


- we apply the chain rule, then collect back into factors $d\mathbf{x}_i$

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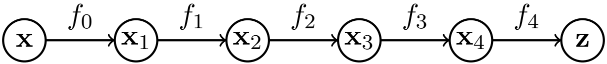
&= d\mathbf{x}_1^\top \cdot Df_0(\mathbf{x}) \\
&= d\mathbf{x}^\top
\end{aligned}
$$

# back-propagation




## forward pass

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

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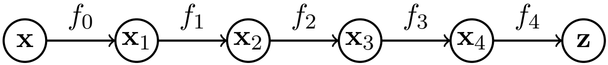


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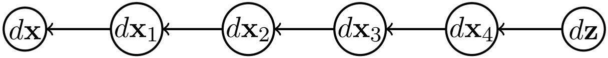


## backward pass

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

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

# 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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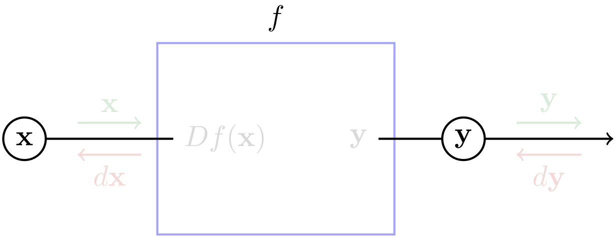
# nodes




- 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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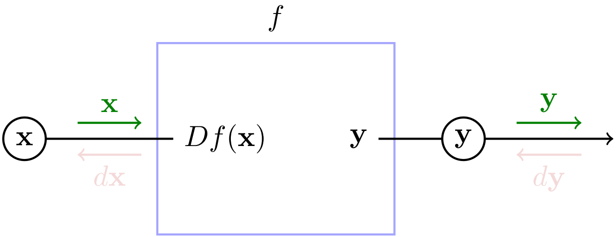


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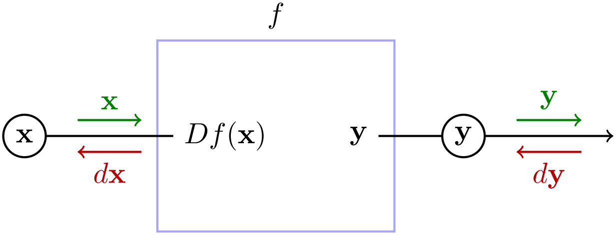


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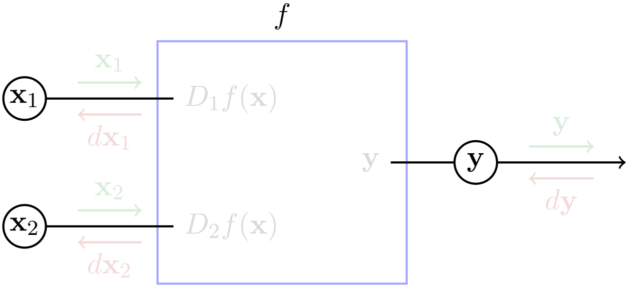
# splitting the input




- 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 $d\mathbf{x}^\top = d\mathbf{y}^\top \cdot Df(\mathbf{x})$ becomes

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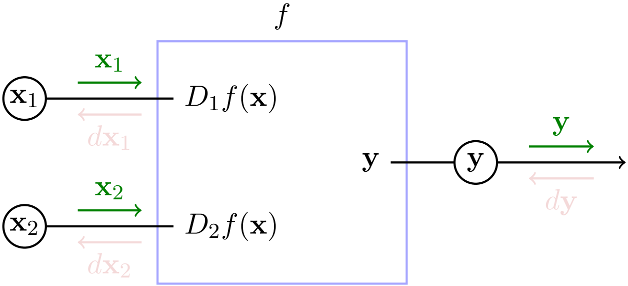


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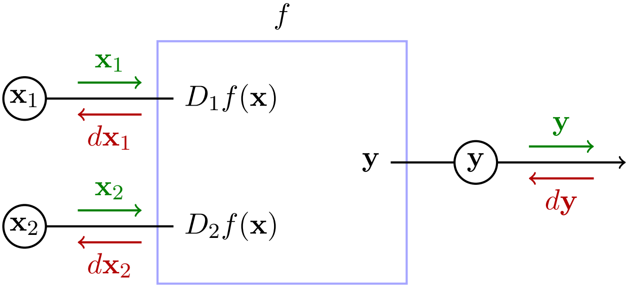


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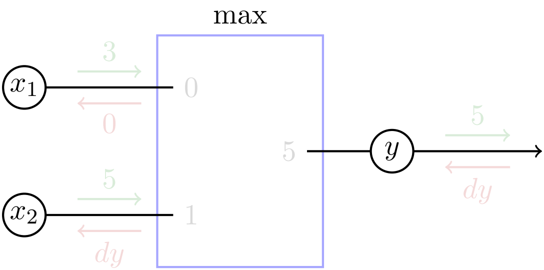
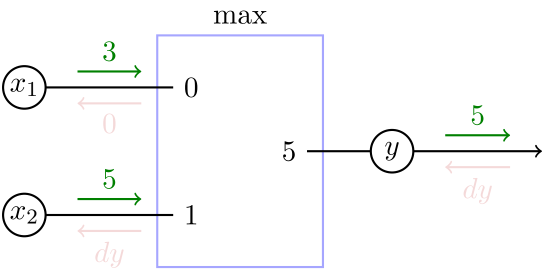
# example: maximum




- 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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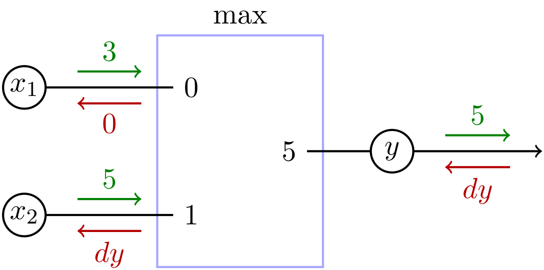


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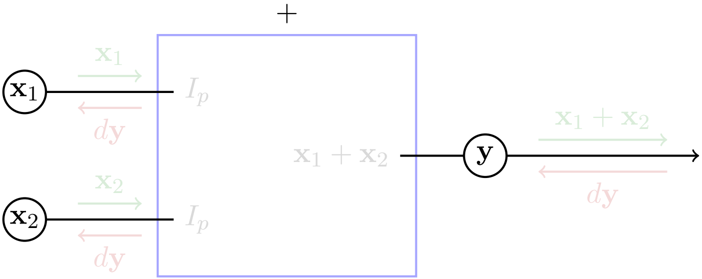
# example: sum




- 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

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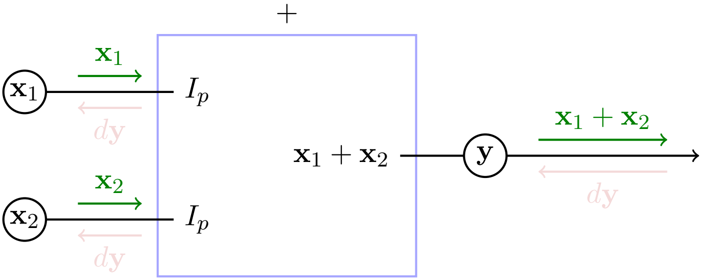


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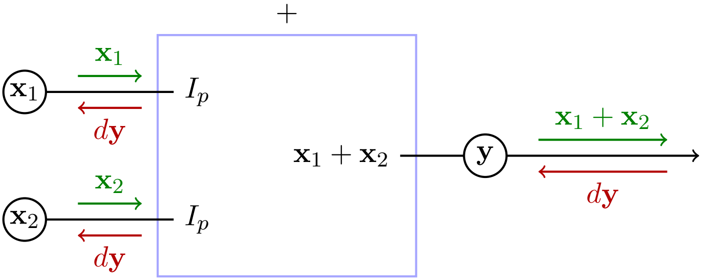


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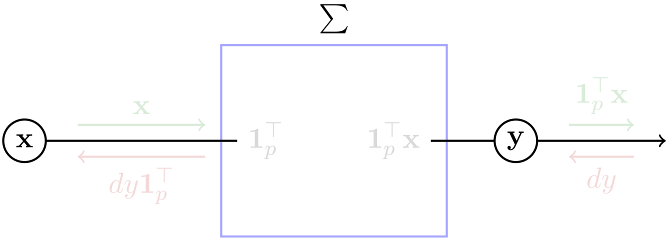
# example: vector sum*




- 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

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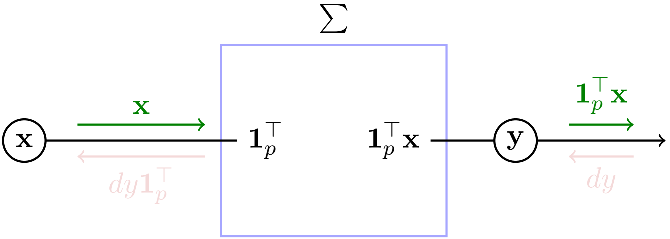


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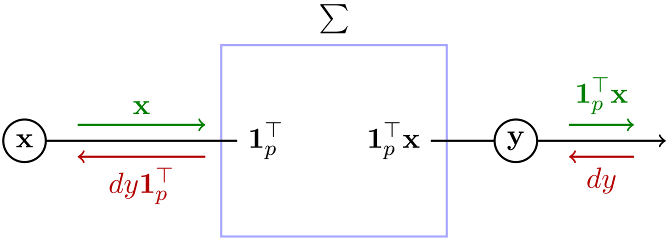


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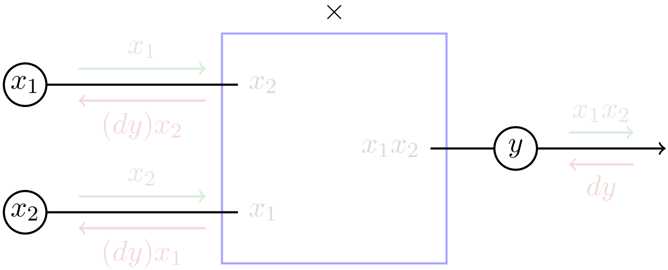
# example: product*

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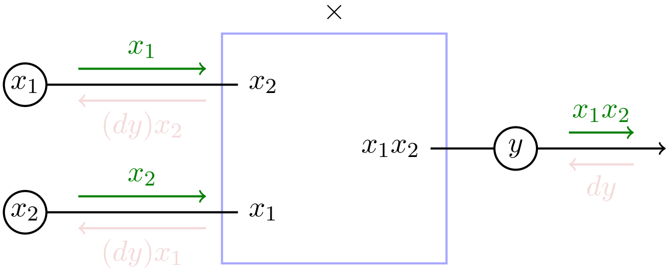


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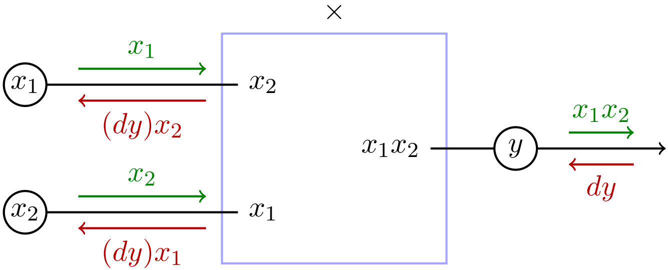


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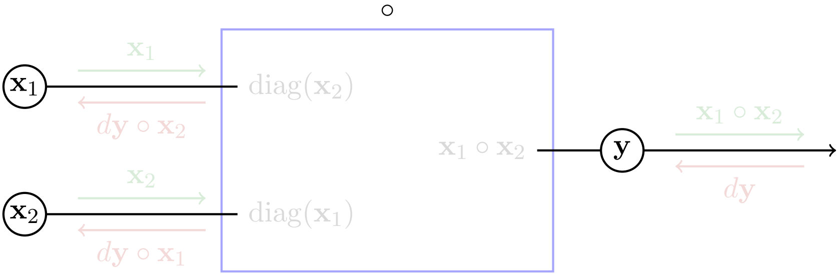
# example: Hadamard (element-wise) product*




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

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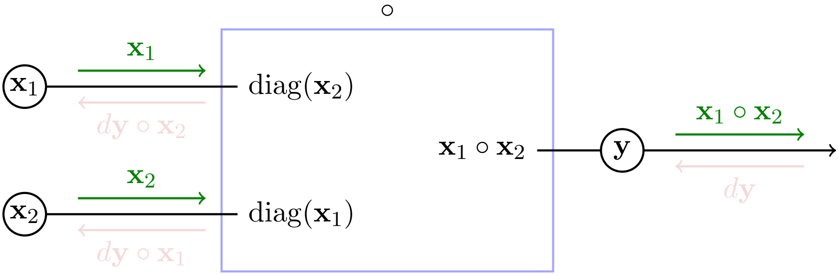


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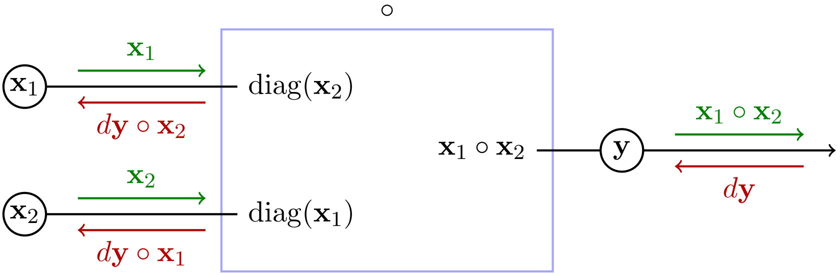


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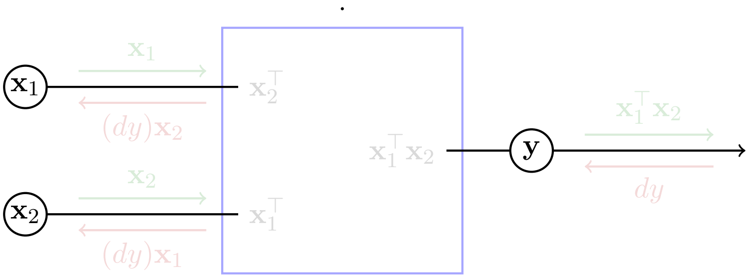


- if $f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1 \cdot \mathbf{x}_2 = \mathbf{x}_1^\top \mathbf{x}_2$, then $D_1 f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_2$ and $D_2 f(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1$
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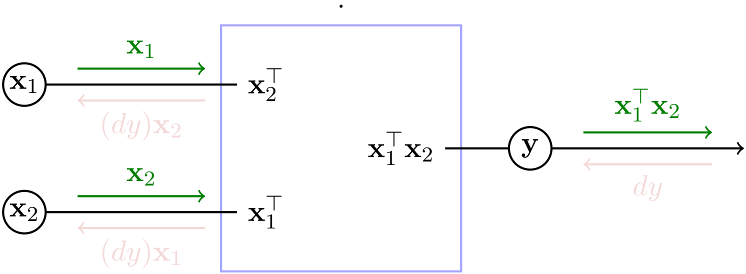


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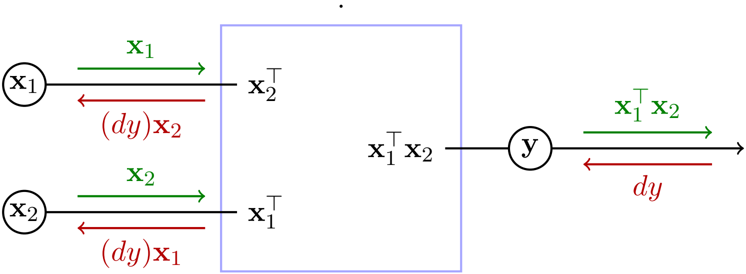


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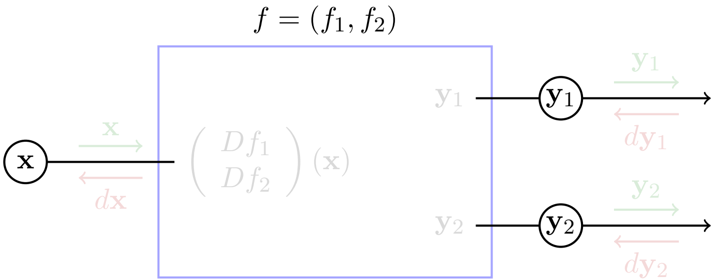
# splitting the output




- 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

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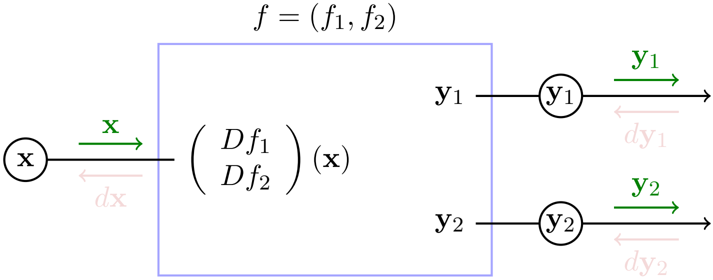


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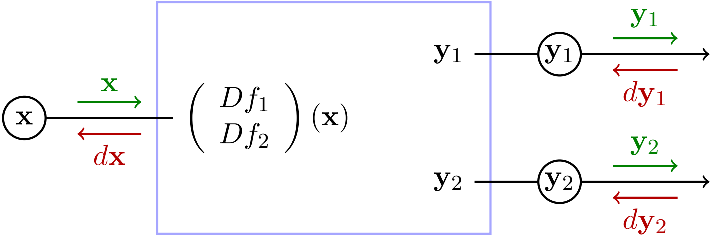
$$Df(\mathbf{x}) = (Df_1; Df_2)(\mathbf{x}) \quad \text{or} \quad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \left( \frac{\partial \mathbf{y}_1}{\partial \mathbf{x}}; \ \frac{\partial \mathbf{y}_2}{\partial \mathbf{x}} \right)$$

- $d\mathbf{y}$ is also split as $d\mathbf{y} = (d\mathbf{y}_1, d\mathbf{y}_2)$ and $d\mathbf{x}^\top = d\mathbf{y}^\top \cdot Df(\mathbf{x})$ 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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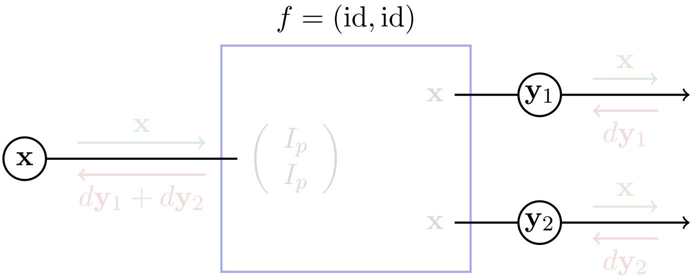
# example: splitter (sharing)




- 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

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

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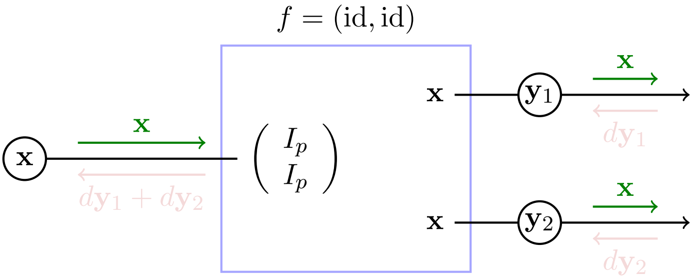


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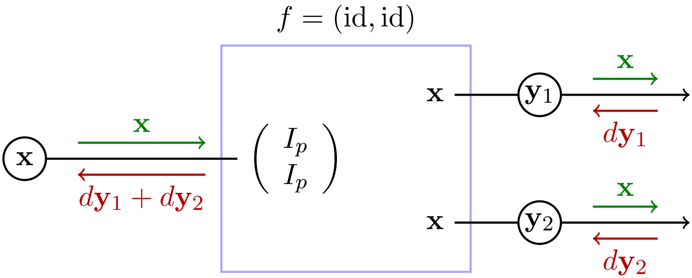


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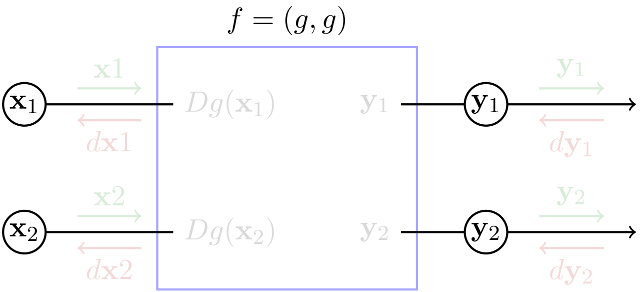
# example: tuples*




- 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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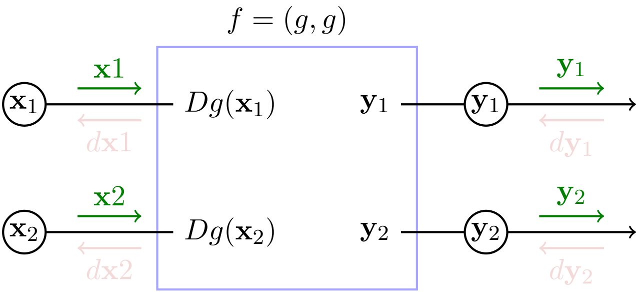


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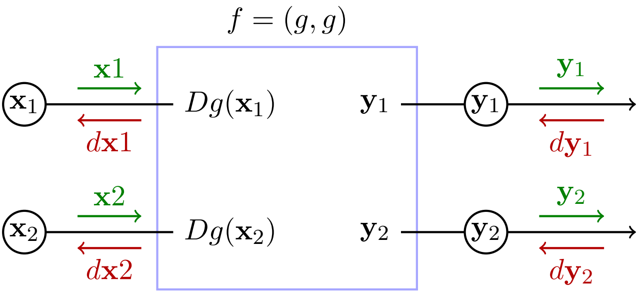


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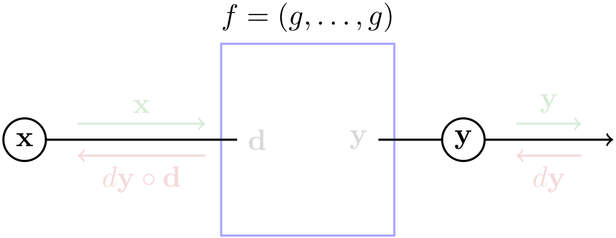
# example: element-wise functions




- 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 $\mathbf{d} = (Dg(x_1), \ldots, Dg(x_p))$
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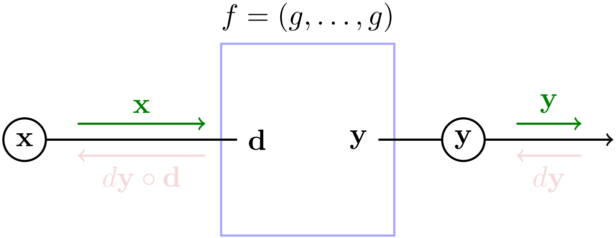


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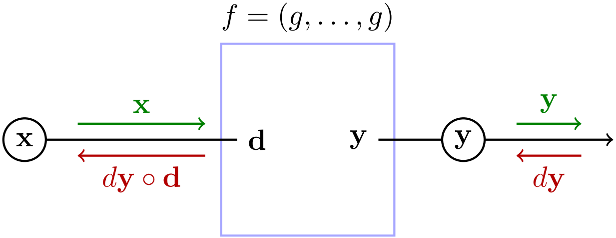


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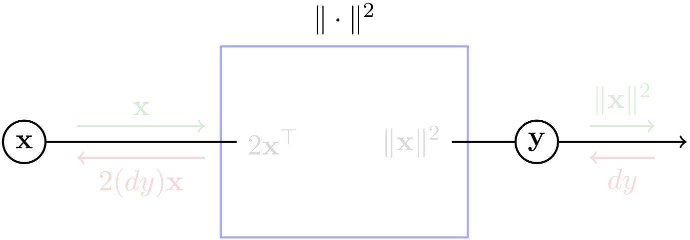
# example: squared norm*




- 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 $\mathbf{x}^\top$)

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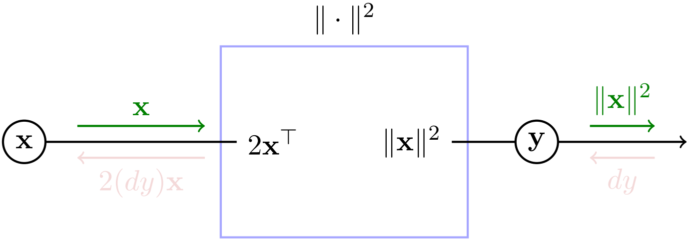


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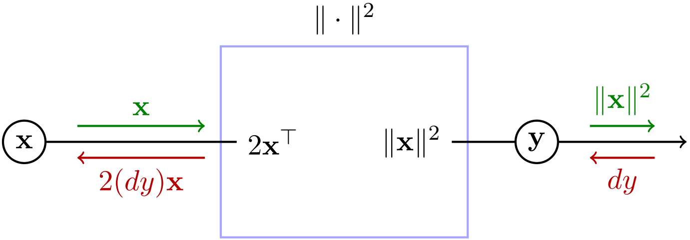


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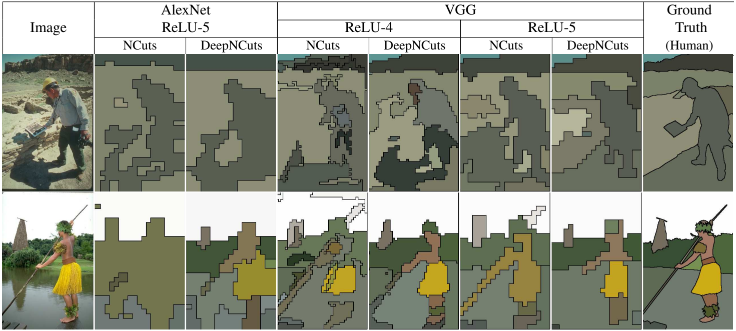
# matrix derivatives*

[Ionescu et al. 2015]




- derivatives for
  - SVD decomposition $A = U\Sigma V^\top$
  - eigenvalue decomposition $A = U\Sigma U^\top$
  - nonlinear matrix functions $f(A) = Uf(\Sigma)U^\top$
- 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

$$\frac{\partial A\mathbf{x}}{\partial \mathbf{x}} = A$$

$$\frac{\partial \mathbf{x}^\top A\mathbf{x}}{\partial \mathbf{x}} = \mathbf{x}^\top (A + A^\top)$$

$$\frac{\partial \mathrm{vec}(\mathbf{x}^\top A\mathbf{x})}{\partial \mathrm{vec}\, A} = \mathbf{x}^\top \otimes \mathbf{x}^\top$$

$$\frac{\partial AXB}{\partial X} = B^\top \otimes A$$

$$\frac{dA^{-1}}{dA} = -(A^{-\top} \otimes A^{-1})$$

$$\frac{d \ln |A|}{dA} = \mathrm{vec}(A^{-\top})^\top$$

$$\frac{\partial \mathrm{tr}(AX)}{\partial X} = \mathrm{vec}(A^\top)^\top$$

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 and the input variables

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

# aside: higher-order derivatives*

- the Hessian was assumed fixed and isotropic in gradient descent; if we knew it, we could use the Newton method instead and solve all curvature-related problems
- given $f : \mathbb{R}^p \to \mathbb{R}$, its Hessian matrix at $\mathbf{x}$ is

$$Hf(\mathbf{x}) := \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_p} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_p \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_p^2} \end{pmatrix} (\mathbf{x}) = \nabla(Df)(\mathbf{x})$$

- unfortunately, this is a $p \times p$ matrix and with $p$ in the order of millions, it is impractical even to store it, let alone compute it

# aside: multiplication by Hessian*

[Pearlmutter 1994]

- fortunately, in many cases what we need is only the product of the Hessian with a given vector $\mathbf{v}$, which is just a vector in $\mathbb{R}^p$

$$\mathbf{v}^\top \cdot Hf(\mathbf{x}) = \mathbf{v}^\top \cdot \nabla(Df)(\mathbf{x}) = \nabla_\mathbf{v}(Df)(\mathbf{x})$$

- here $\nabla_\mathbf{v}$ is the directional derivative operator

$$\nabla_\mathbf{v}(f) := \mathbf{v}^\top \cdot \nabla f$$

- remember that in back-propagation, for each variable $\mathbf{x}$, we defined a vector $d\mathbf{x}$, which was computed in the backward pass
- so all we need to do is allocate another vector $\nabla_\mathbf{v}(\mathbf{x})$ for the forward pass and another $\nabla_\mathbf{v}(d\mathbf{x})$ for the backward, and compute them by applying the chain rule in both passes!

Pearlmutter. NC 1994. Fast Exact Multiplication By the Hessian.

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# 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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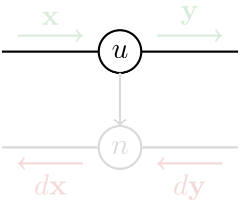
# units and nodes




- unit $u$ manually generates node $n$

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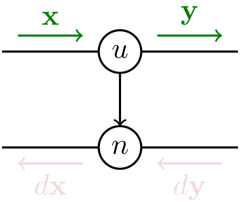


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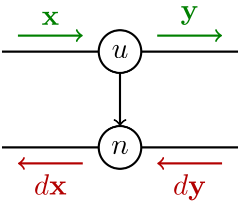


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# units and nodes

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

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

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

**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** $node(A, \text{back})$

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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 $A$, $W$,

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

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 $W$

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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

# the affine unit in math*

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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

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

# 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 logic 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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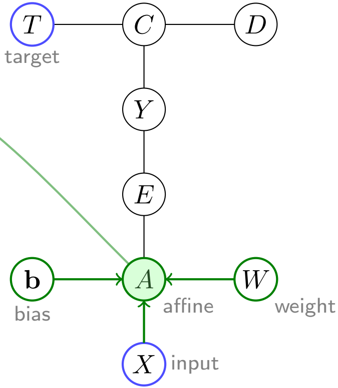
# back-propagation

**forward**

$A = \text{dot}(X, W) + \mathbf{b}$



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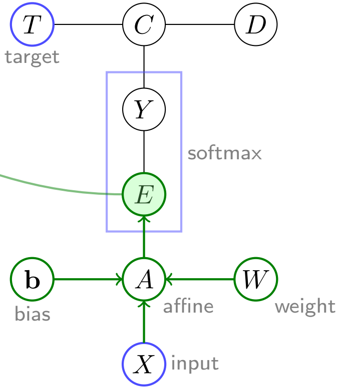

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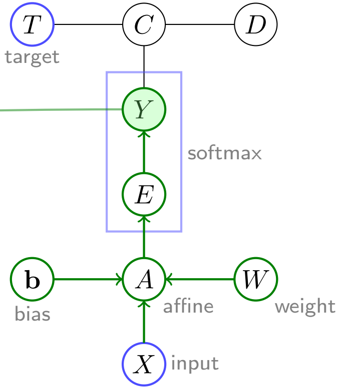

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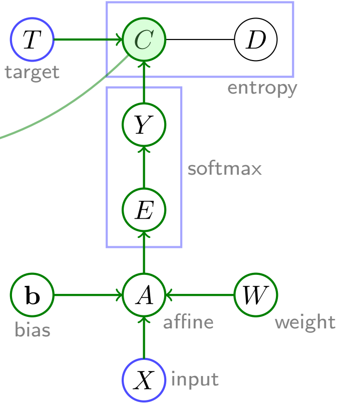

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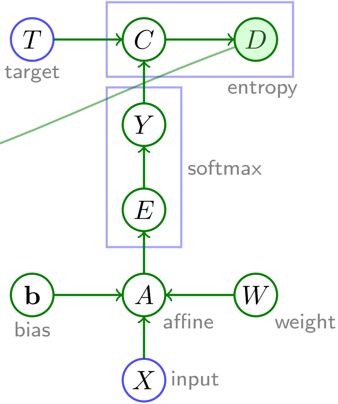

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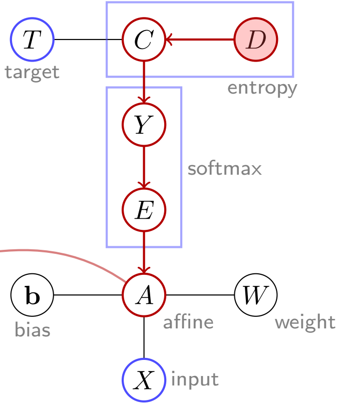
$dA = dD * (Y - T)/m$



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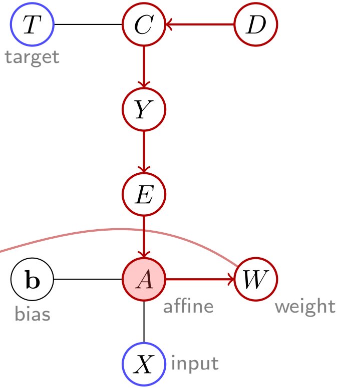
**backward**

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



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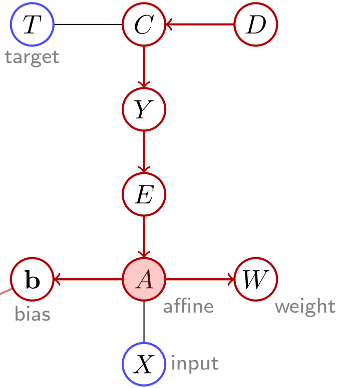
**backward**

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



# automatic differentiation

**forward**

$$A = \mathrm{dot}(X, W) + \mathbf{b}$$
$$E = \exp(A)$$
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**backward**

$$dA = dD * (Y - T)/m$$
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now we organize forward and backward code into units

# automatic differentiation

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

**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** $\mathit{node}(A, \text{back})$

# automatic differentiation

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$D = \text{sum}_0(C)/m$

**backward**

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

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**def** $\text{back}(dD, dA, \_)$:
$dA \mathrel{+}= dD * (Y - T)/m$
**return** $\textit{node}(D, \text{back})$

# automatic differentiation

**forward**

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

$D = \text{entropy}(A, T)$

```
def logistic(A, T):
    E = exp(A)
    Y = E / sum_1(E)
    C = -sum_1(T * log(Y))
    D = sum_0(C) / m
    def back(dD, dA, _):
        dA += dD * (Y - T) / m
    return node(D, back)
```

**backward**

$D.\text{back}(A, T)$

$A.\text{back}(X, (W, \mathbf{b}))$

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

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\end{aligned}
$$

# the decay unit*

- it takes as input a tuple or list $W$ of weight matrices 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 $\ell_2$ 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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    return node(R, back)
```

# the add unit*

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

```
def add(X):
    S = sum(X)
    def back(dS, dX):
        for dx in dX:
            dx += dS
    return node(S, back)
```

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

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# the $\mathrm{loss}$ function

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

$$
\begin{array}{l}
\textbf{def } \mathrm{loss}(A, T, W): \\
\quad L = \mathrm{logistic}(A, T) + \mathrm{decay}(W) \\
\quad \textbf{return } \mathit{block}(L)
\end{array}
$$

- addition is handled by $\mathrm{add}$ and the error derivative flows backward to both branches

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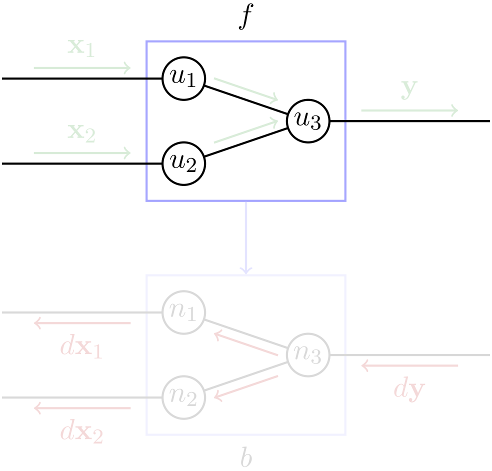
# the model function

- this is a two-layer network model where an affine layer is followed by a $\mathrm{relu}$ 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

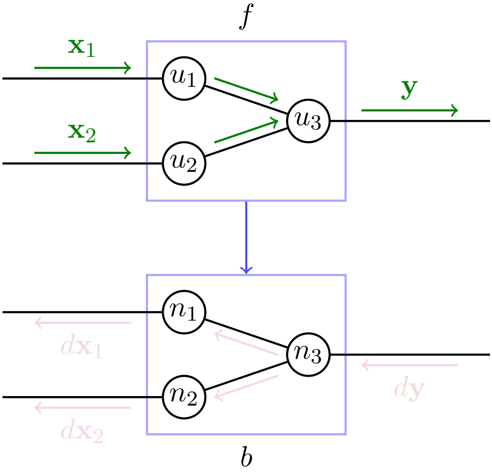
$$
\begin{array}{l}
\textbf{def } \mathrm{model}(X, (U_1, U_2)): \\
\quad A = \mathrm{affine}(\mathrm{relu}(\mathrm{affine}(X, U_1)), U_2) \\
\quad \textbf{return } \mathit{block}(A)
\end{array}
$$

# 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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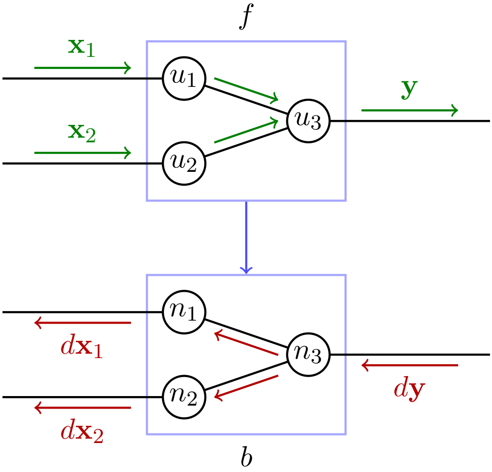


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# functions and blocks

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

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

- all calls are recorded as a list of *unit*s or *function*s 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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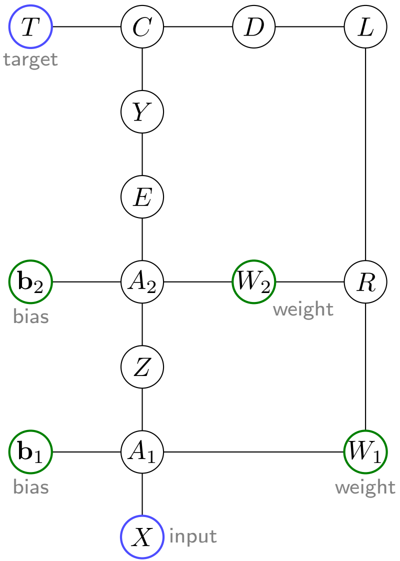
$$
\begin{aligned}
&\textbf{def } name(\mathbf{x}_1, \ldots, \mathbf{x}_n):\\
&\quad \langle\text{code generating the following}\rangle\\
&\quad \mathbf{r}_1 = \text{call}_1(\mathbf{a}_1, \ldots, \mathbf{a}_{n_1})\\
&\qquad \vdots\\
&\quad \mathbf{r}_s = \text{call}_s(\mathbf{a}_1, \ldots, \mathbf{a}_{n_s})\\
&\quad \textbf{return } block(\mathbf{r}_s)
\end{aligned}
$$

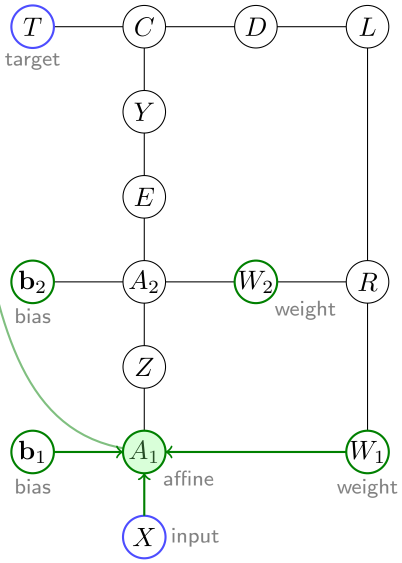
- all calls are recorded as a list of *unit*s or *function*s by call order, each associated with a list of arguments
- a *block* object is a *node*, but
  - its method back() does not add its own derivative in the arguments
  - its method back() is automatically generated and its body calls the recorded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

# back-propagation



# back-propagation

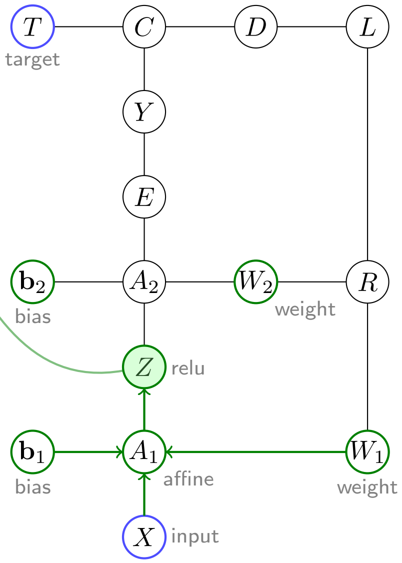
$$A_1 = \textcolor{blue}{\mathrm{dot}}(X, W_1) + \mathbf{b}_1$$



# back-propagation

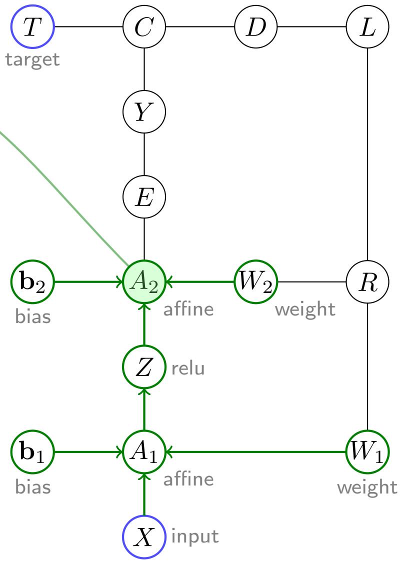
$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$

$Z = \max(0, A_1)$



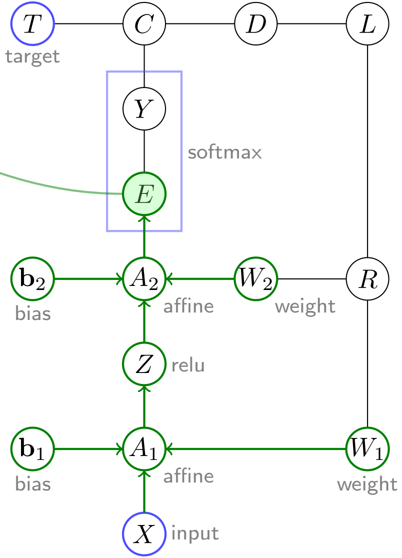
# back-propagation

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



# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
$Z = \text{max}(0, A_1)$
$A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2$
$E = \text{exp}(A_2)$
$Y = E/\text{sum}_1(E)$
$C = -\text{sum}_1(T * \text{log}(Y))$
$D = \text{sum}_0(C)/m$



# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
$Z = \max(0, A_1)$
$A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2$
$E = \exp(A_2)$
$Y = E/\text{sum}_1(E)$
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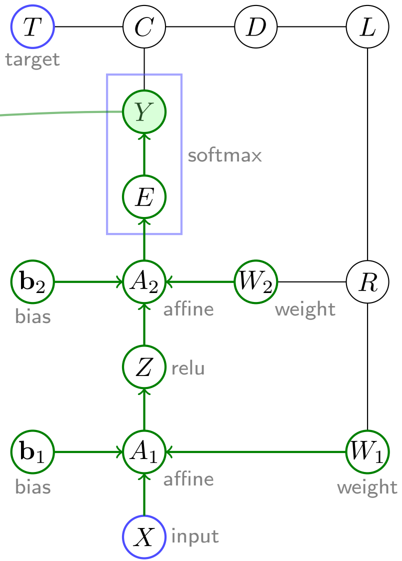

# back-propagation

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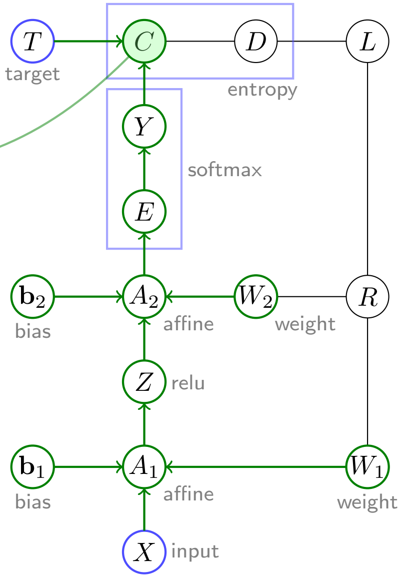

# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
$Z = \max(0, A_1)$
$A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2$
$E = \exp(A_2)$
$Y = E/\text{sum}_1(E)$
$C = -\text{sum}_1(T * \log(Y))$
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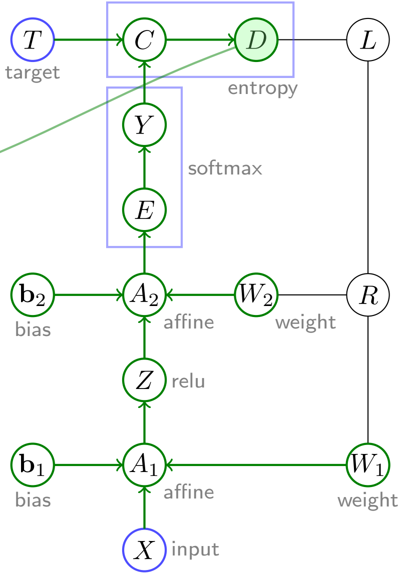

# back-propagation

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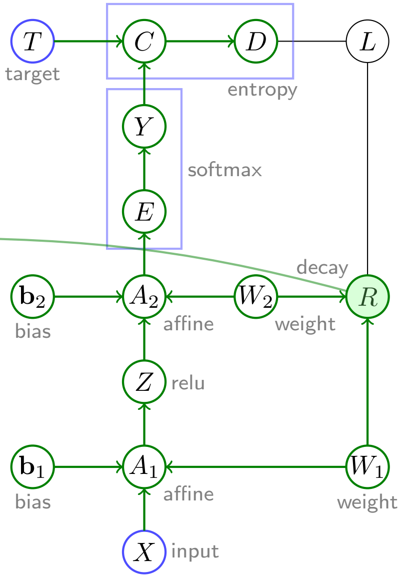
$$E = \exp(A_2)$$
$$Y = E/\text{sum}_1(E)$$
$$C = -\text{sum}_1(T * \log(Y))$$
$$D = \text{sum}_0(C)/m$$
$$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$$



# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
$Z = \text{max}(0, A_1)$
$A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2$
$E = \text{exp}(A_2)$
$Y = E/\text{sum}_1(E)$
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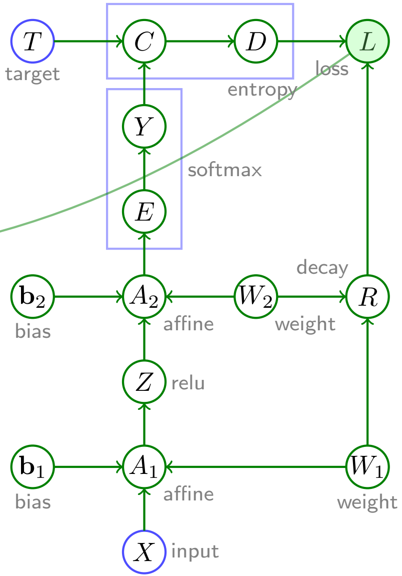
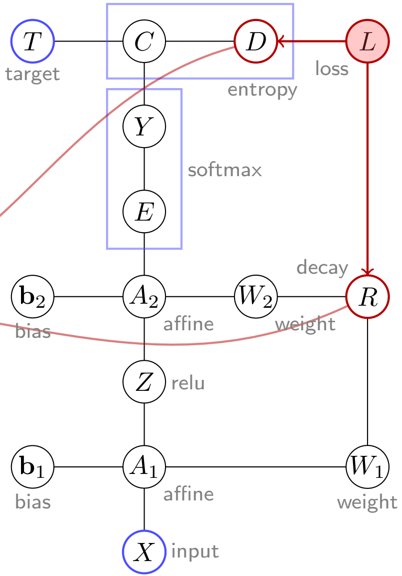
$D = \text{sum}_0(C)/m$
$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$
$L = D + R$



# back-propagation

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



# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
$Z = \max(0, A_1)$
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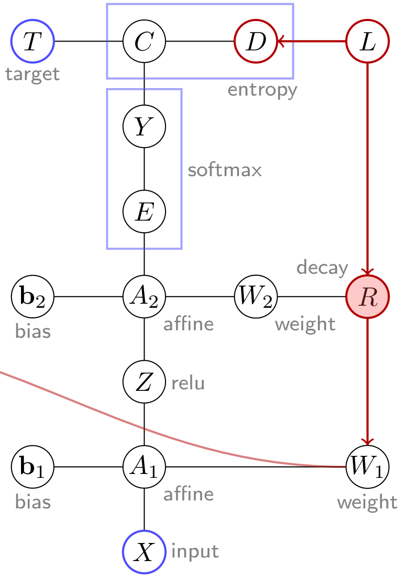
$L = D + R$
$(dD, dR) = (dL, dL)$
$dW_1 = dR * \lambda * W_1$
$dW_2 = dR * \lambda * W_2$



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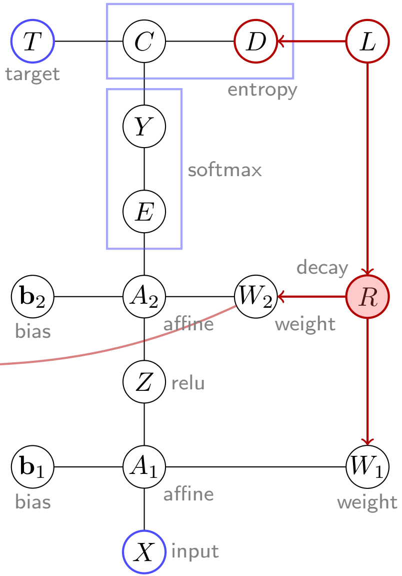
$Y = E / \textcolor{blue}{\text{sum}_1}(E)$
$C = -\textcolor{blue}{\text{sum}_1}(T * \textcolor{blue}{\log}(Y))$
$D = \textcolor{blue}{\text{sum}_0}(C)/m$
$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$
$L = D + R$

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



# back-propagation

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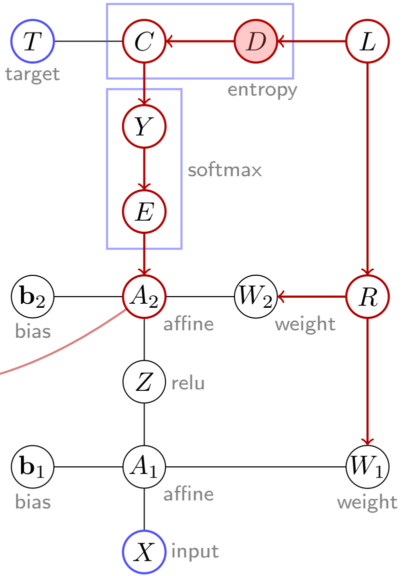
$D = \text{sum}_0(C)/m$
$R = \frac{\lambda}{2} * (\|W_1\|_F^2 + \|W_2\|_F^2)$
$L = D + R$
$(dD, dR) = (dL, dL)$
$dW_1 = dR * \lambda * W_1$
$dW_2 = dR * \lambda * W_2$
$dA_2 = dD * (Y - T)/m$



# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
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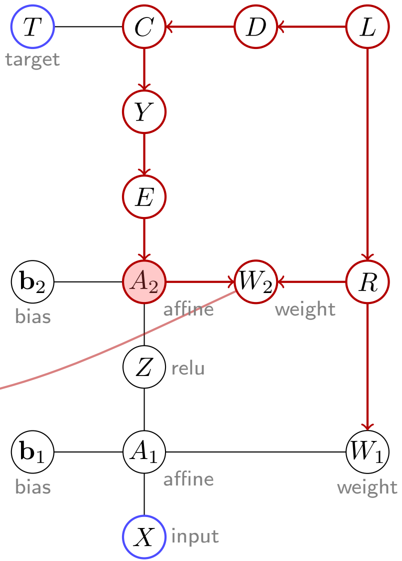
$(dD, dR) = (dL, dL)$
$dW_1 = dR * \lambda * W_1$
$dW_2 = dR * \lambda * W_2$
$dA_2 = dD * (Y - T)/m$
$dW_2 \mathrel{+}= \text{dot}(Z^\top, dA_2)$
$d\mathbf{b}_2 = \text{sum}_0(dA_2)$
$dZ = \text{dot}(dA_2, W_2^\top)$



# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
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$d\mathbf{b}_2 = \text{sum}_0(dA_2)$
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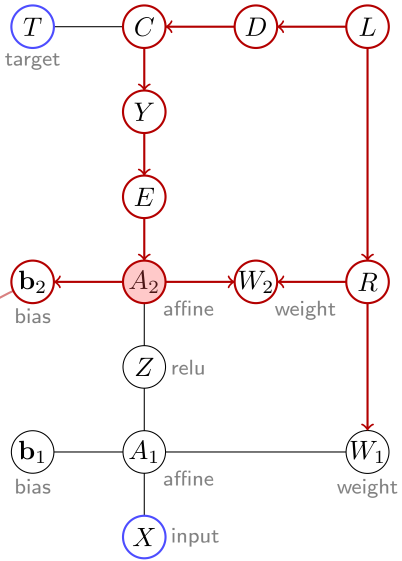

# back-propagation

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$Z = \max(0, A_1)$
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$dA_2 = dD * (Y - T)/m$
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$d\mathbf{b}_2 = \text{sum}_0(dA_2)$
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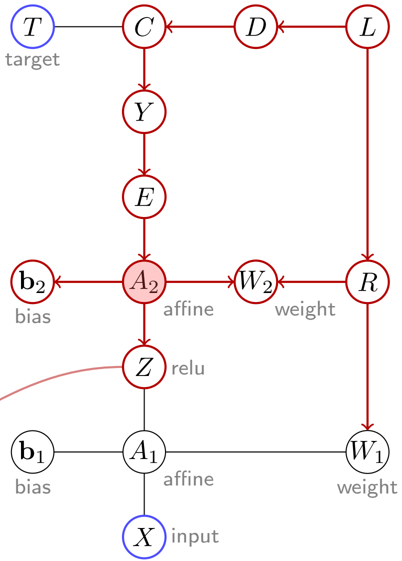

# back-propagation

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$Z = \max(0, A_1)$
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$dW_1 = dR * \lambda * W_1$
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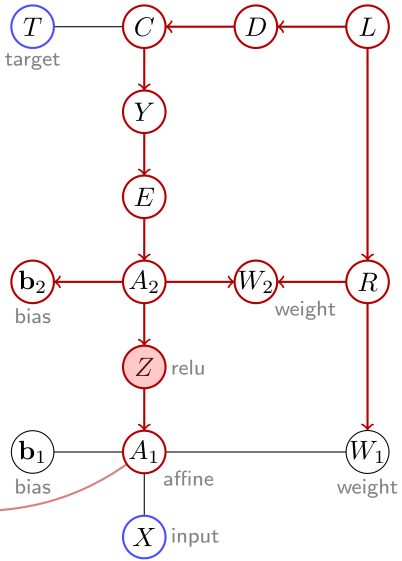
$dA_2 = dD * (Y - T)/m$
$dW_2 \mathrel{+}= \text{dot}(Z^\top, dA_2)$
$d\mathbf{b}_2 = \text{sum}_0(dA_2)$
$dZ = \text{dot}(dA_2, W_2^\top)$
$dA_1 = dZ * (Z > 0)$



# back-propagation

$A_1 = \text{dot}(X, W_1) + \mathbf{b}_1$
$Z = \max(0, A_1)$
$A_2 = \text{dot}(Z, W_2) + \mathbf{b}_2$
$E = \exp(A_2)$
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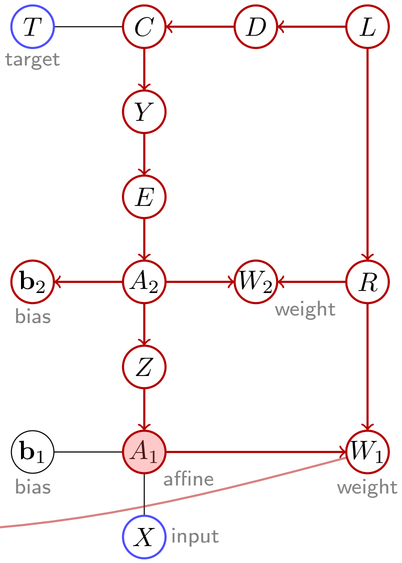
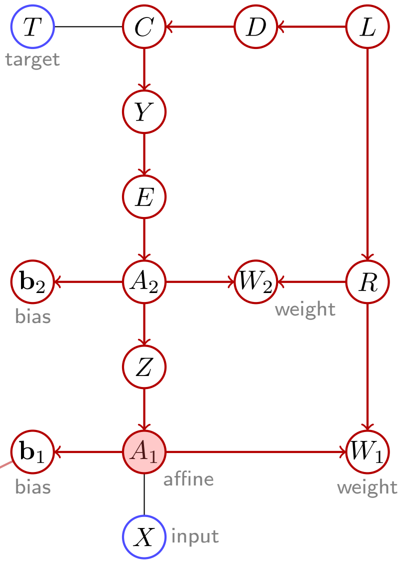
$dZ = \text{dot}(dA_2, W_2^\top)$
$dA_1 = dZ * (Z > 0)$
$dW_1 \mathrel{+}= \text{dot}(X^\top, dA_1)$
$d\mathbf{b}_1 = \text{sum}_0(dA_1)$



# back-propagation

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



# automatic differentiation

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

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

now we organize forward and backward code into units and functions

# automatic differentiation

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

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

# automatic differentiation

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

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

# automatic differentiation

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

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

**def** $\text{affine}(X, (W, \mathbf{b}))$:
  $A = \text{dot}(X, W) + \mathbf{b}$
  **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** $\textit{node}(A, \text{back})$

# automatic differentiation

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

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

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

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

# automatic differentiation

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

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

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

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

# 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 = 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)
```

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

# 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** $\mathit{block}(L, \text{back})$

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

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

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

# automatic differentiation

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

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

**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** $\mathit{block}(L, \text{back})$

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

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

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

# 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** $\text{model}(X, (U_1, U_2))$:
  $A_1 = \text{affine}(X, U_1)$
  $Z = \text{relu}(A)$
  $A_2 = \text{affine}(Z, U_2)$
  **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** $\mathit{block}(A_2, \text{back})$

# 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** $\mathit{block}(A_2, \text{back})$

# 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** $\mathit{block}(A)$

**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** $\mathit{block}(A_2, \text{back})$

# pynet

code available at https://github.com/iavr/pynet

# deep learning software

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

# 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 units (forward) and nodes (backward)
- grouping into functions (forward) and blocks (backward)