Training DNNs: Basic Methods

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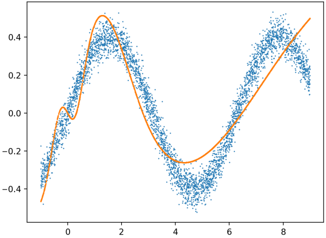
Supervised learning as function approximation



- Underlying true function: f_0
- Training data: $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}$ with $\boldsymbol{y}_i \approx f_0(\boldsymbol{x}_i)$
- Choose a family of functions $\mathcal{H}$, so that $\exists f \in \mathcal{H}$ and f and f_0 are close
- Find f, i.e., optimization

$$\min_{f \in \mathcal{H}} \sum_i \ell(\boldsymbol{y}_i, f(\boldsymbol{x}_i)) + \Omega(f)$$

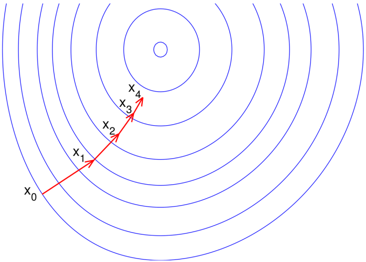
- **Approximation capacity: Univeral approximation theorems (UAT)** $\Longrightarrow$ replace $\mathcal{H}$ by $\mathrm{DNN}_{\boldsymbol{W}}$, i.e., a deep neural network with weights $\boldsymbol{W}$
- **Optimization:**

$$\min_{\boldsymbol{W}} \sum_i \ell(\boldsymbol{y}_i, \mathrm{DNN}_{\boldsymbol{W}}(\boldsymbol{x}_i)) + \Omega(\boldsymbol{W})$$

- **Generalization:** how to avoid over-complicated $\mathrm{DNN}_{\boldsymbol{W}}$ in view of UAT

Basics of numerical optimization

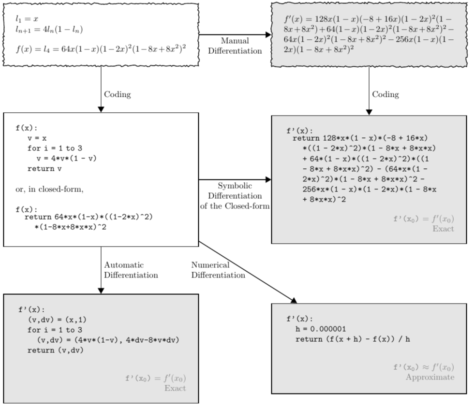
- 1st and 2nd optimality conditions
- iterative methods



Credit: aria42.com

- gradient descent
- Newton's method
- momentum methods
- quasi-Newton methods
- coordinate descent
- conjugate gradient methods
- trust-region methods
- etc

Computing derivatives



Credit: [Baydin et al., 2017]

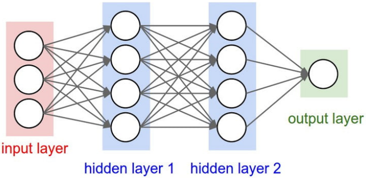
- Analytic differentiation (by hand or by software)
- Finite difference approximation
- Automatic/Algorithmic differentiation (AD)

Ready to optimize DNNs!

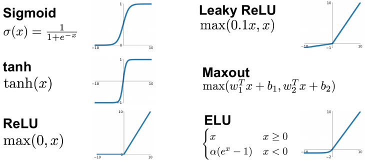
Outline

Set up the problem

DNN



activation function



Credit: Stanford CS231N

Set up the problem

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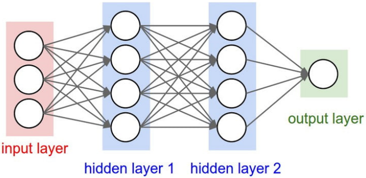

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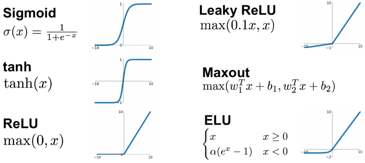

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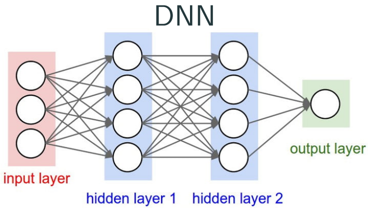

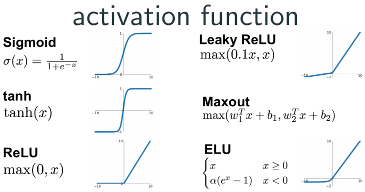

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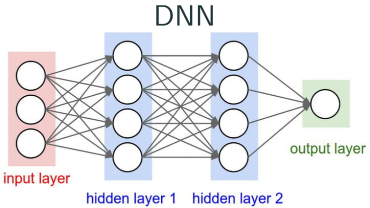
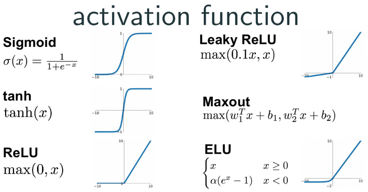
– Which activation at the hidden nodes?

Set up the problem





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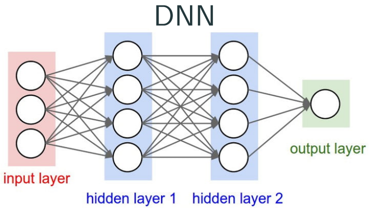

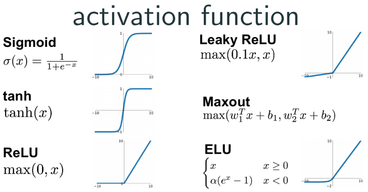

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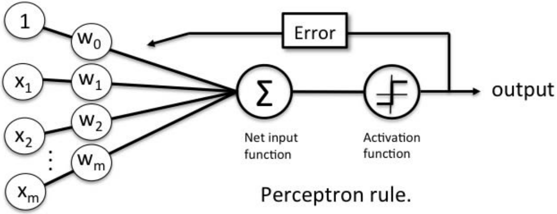

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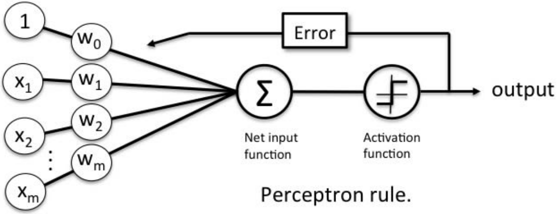

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$$\nabla_{\boldsymbol{w}} \ell \left(\text{sign}\left(\boldsymbol{w}^\intercal \boldsymbol{x}\right), y\right) = \ell' \left(\text{sign}\left(\boldsymbol{w}^\intercal \boldsymbol{x}\right), y\right) \text{sign}'\left(\boldsymbol{w}^\intercal \boldsymbol{x}\right) \boldsymbol{x} = \mathbf{0}$$

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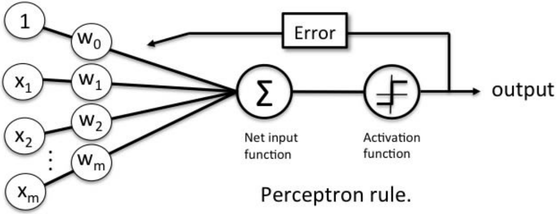

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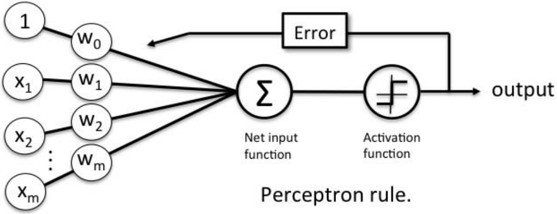

Perceptron rule.

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Desiderata:

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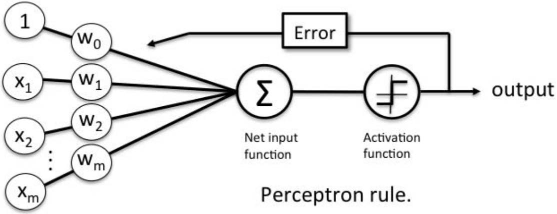

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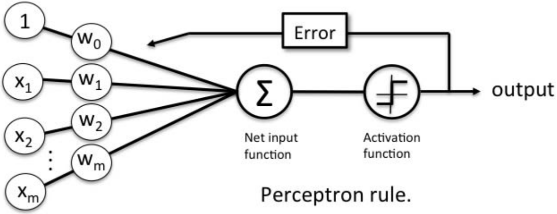

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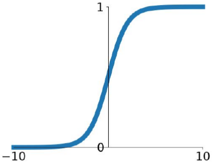
Sigmoid and hypertangent



Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

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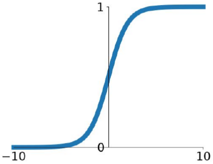

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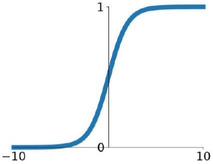

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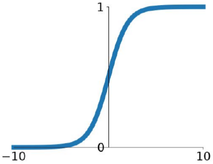

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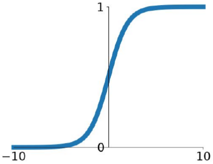

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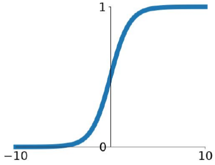

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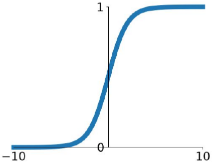

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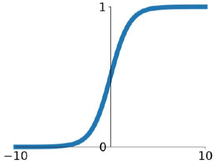

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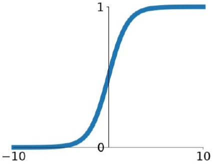

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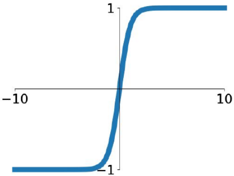
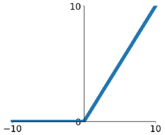
What about $\tanh$?



tanh(x)

ReLU and friends



ReLU
(Rectified Linear Unit)

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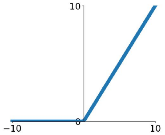

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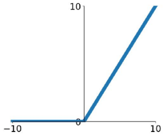

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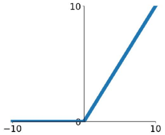

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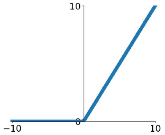

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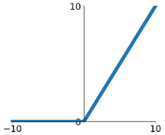

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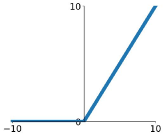

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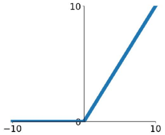

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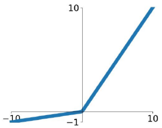

Leaky ReLU

$$\sigma(x) = \max(\alpha x, x) \quad \text{(e.g., } \alpha = 0.01\text{)}$$

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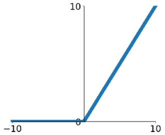

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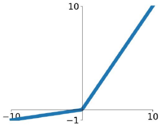

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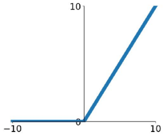

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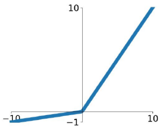

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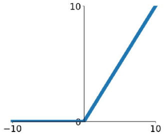

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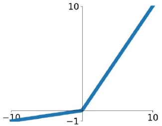

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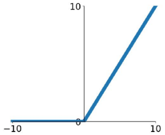

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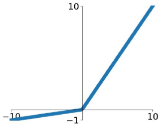

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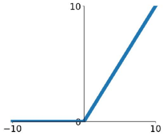

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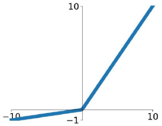
- Nonzero derivatives? **Yes and No!** What happens for $x < 0$?
- Cheap? **Yes!**



Leaky ReLU

$$\sigma(x) = \max(\alpha x, x) \qquad (\text{e.g., } \alpha = 0.01)$$

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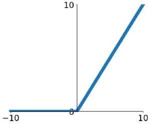
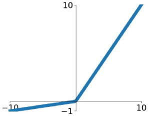
ReLU and friends

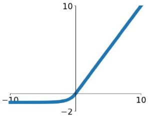


ReLU
(Rectified Linear Unit)



Leaky ReLU

Exponential Linear Units (ELU)



$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$

– ReLU and Leaky ReLU are the most popular

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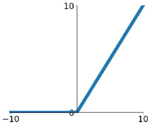

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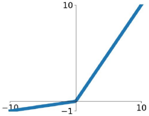

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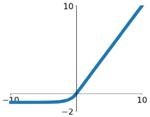

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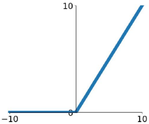

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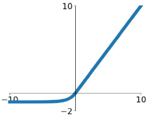

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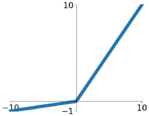

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- ReLU and Leaky ReLU are the most popular
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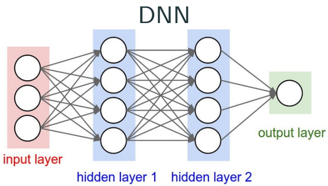
- Question: what do you think of $|\cdot|$ as activation?

Which activation at output node?



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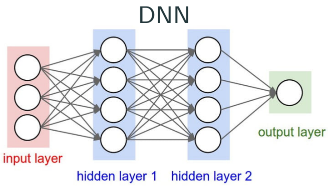

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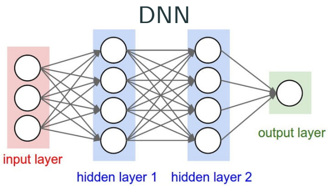

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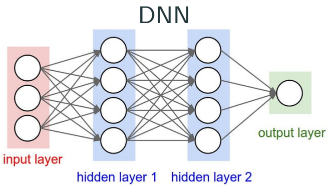

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$$L_k \Longrightarrow [\underbrace{0, \ldots, 0,}_{k-1\, 0's}, 1, \underbrace{0, \ldots, 0}_{n-k\, 0's}]^\intercal$$

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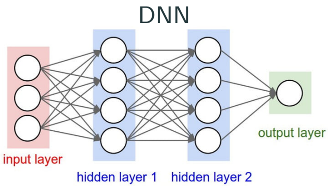

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- discrete probability distribution: softmax
- etc .

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Which ℓ to choose? Make it differentiable, or almost so

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- **difference between distributions**: Kullback-Leibler divergence loss (`torch.nn.KLDivLoss`) or Wasserstein metric

Outline

Three design choices

Training algorithms

- Which method
- Where to start
- When to stop

Suggested reading

Framework of line-search methods

A generic line search algorithm

Input: initialization $\boldsymbol{x}_0$, stopping criterion (SC), $k = 1$

while SC not satisfied **do**
    choose a direction $\boldsymbol{d}_k$
    decide a step size t_k
    make a step: $\boldsymbol{x}_k = \boldsymbol{x}_{k-1} + t_k \boldsymbol{d}_k$
    update counter: $k = k + 1$
end while

Four questions:

- How to choose direction $\boldsymbol{d}_k$?
- How to choose step size t_k?
- Where to initialize?
- When to stop?

Outline

From deterministic to stochastic optimization

Recall our optimization problem:

$$\min_{\boldsymbol{W}} \frac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right) + \Omega\left(\boldsymbol{W}\right)$$

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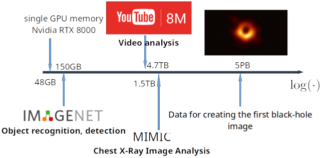

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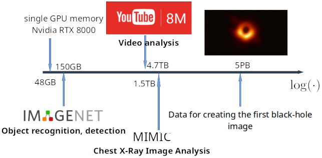

- **computation**: each iteration costs at least $O(mn)$, where n is #(opt variables)—both can be large for training DNNs!

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How to get around the storage and computation bottleneck when m is large?

stochastic optimization (stochastic = random)

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... justified by the law of large numbers

Stochastic gradient descent (SGD)

In general (i.e., not only for DNNs), suppose we want to solve

$$\min_{\boldsymbol{w}} \; F(\boldsymbol{w}) \doteq \frac{1}{m} \sum_{i=1}^{m} f(\boldsymbol{w}; \boldsymbol{\xi}_i) \qquad \xi_i\text{'s are data samples}$$

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Input: initialization $\boldsymbol{x}_0$, stopping criterion (SC), $k = 1$

1: **while** SC not satisfied **do**

2: sample a random subset $J_k \subset \{0, \dots, m-1\}$

3: calculate the stochastic gradient $\widehat{\boldsymbol{g}_k} \doteq \frac{1}{|J_k|} \sum_{j \in J_k} \nabla_{\boldsymbol{w}} f(\boldsymbol{w}; \boldsymbol{\xi}_i)$

4: decide a step size t_k

5: make a step: $\boldsymbol{x}_k = \boldsymbol{x}_{k-1} - t_k \widehat{\boldsymbol{g}_k}$

6: update counter: $k = k + 1$

7: **end while**

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- J_k is redrawn in each iteration
- Traditional SGD: $|J_k| = 1$. The version presented is also called **mini-batch gradient descent**

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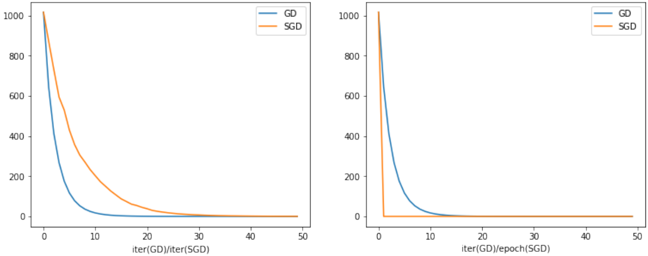
Practical stochastic gradient descent (SGD)

Input: init. $\boldsymbol{x}_0$, SC, batch size B, iteration counter $k = 1$, epoch counter $\ell = 1$

```
while SC not satisfied do
    permute the index set {0, ··· , m} and divide it into batches of size B
    for i ∈ {1, ..., #batches} do
        calculate the stochastic gradient ĝ_k based on the i^th batch
        decide a step size t_k
        make a step: x_k = x_{k−1} − t_k ĝ_k
        update iteration counter: k = k + 1
    end for
    update epoch counter: ℓ = ℓ + 1
end while
```

GD vs. SGD

Consider $\min_{\boldsymbol{w}} \; \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2$, where $\boldsymbol{X} \in \mathbb{R}^{10000\times 500}$, $\boldsymbol{y} \in \mathbb{R}^{10000}$, $\boldsymbol{w} \in \mathbb{R}^{500}$



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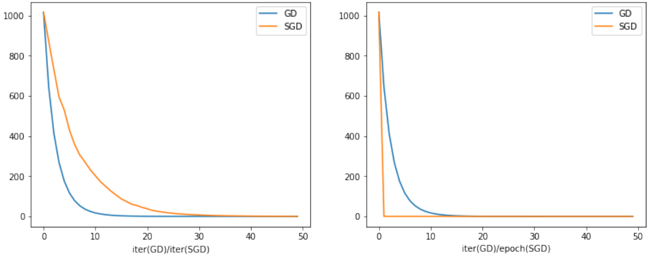

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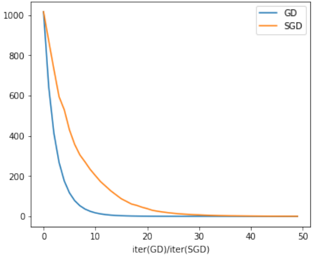

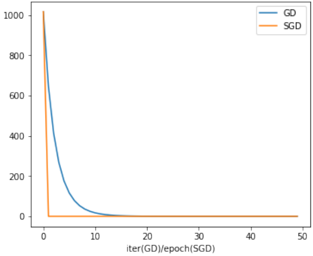

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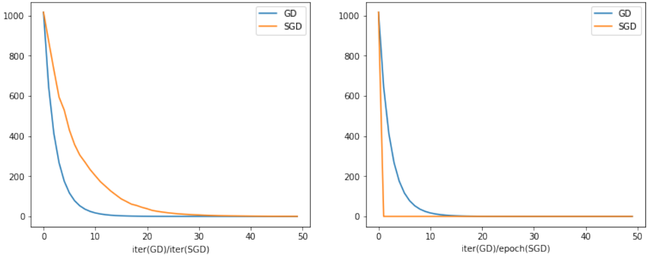

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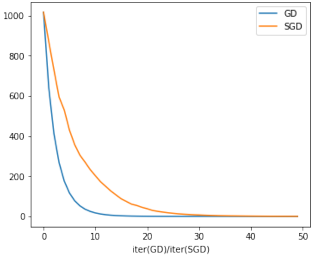

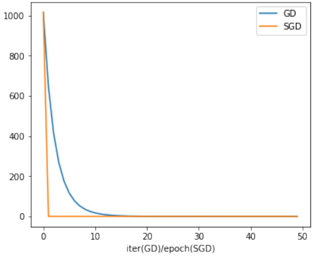

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Overall, SGD could be quicker to find a medium-accuracy solution with lower cost, which suffices for most purposes in machine learning [Bottou and Bousquet, 2008].

Step size (learning rate) for SGD

Recall the recommended step size rule for GD: **back-tracking line search**

key idea: $F\left(\boldsymbol{x} - t\nabla F\left(\boldsymbol{x}\right)\right) - F\left(\boldsymbol{x}\right) \approx -ct\left\|\nabla F\left(\boldsymbol{x}\right)\right\|^2$ for a certain $c \in (0, 1)$

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- What about computing approximations to the objective values based on small batches also? Approximation errors for F and ∇F may ruin the stability of the Taylor criterion

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$$\sum_k t_k = \infty, \quad \sum_k t_k^2 < \infty.$$

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check out `torch.optim.lr_scheduler` in PyTorch! https://pytorch.org/docs/stable/optim.html#how-to-adjust-learning-rate

Beyond the vanilla SGD

– Momentum/acceleration methods

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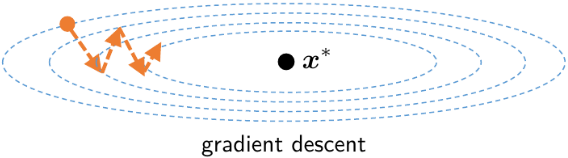
- Stochastic 2nd order methods

Why momentum?



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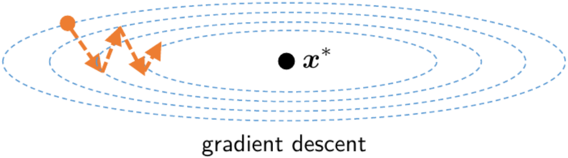

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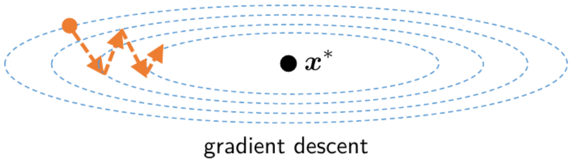

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A cheap way to achieve faster convergence? Answer: using historic information

Heavy ball method

In physics, a heavy object has a large inertia/momentum — resistance to change velocity.

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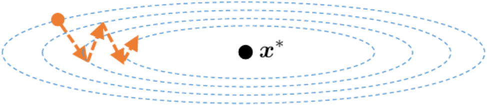
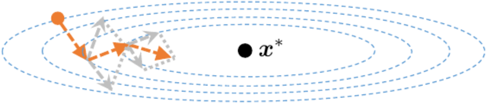


gradient descent



heavy-ball method

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History helps to smooth out the zig-zag path!

Nesterov's accelerated gradient methods

due to Y. Nesterov

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \beta_k \left(\boldsymbol{x}_k - \boldsymbol{x}_{k-1}\right) - \alpha_k \nabla f \left(\boldsymbol{x}_k + \beta_k \left(\boldsymbol{x}_k - \boldsymbol{x}_{k-1}\right)\right)$$

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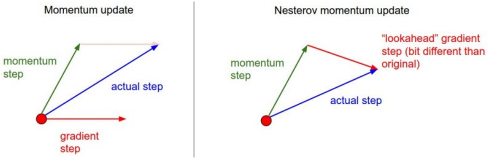

Credit: Stanford CS231N

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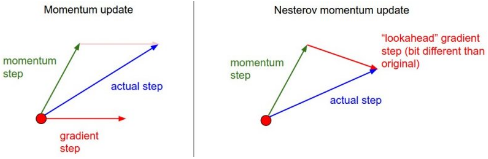

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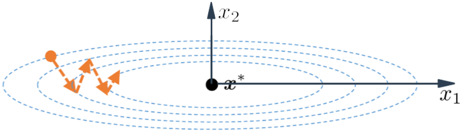
SGD with momentum/acceleration: replace the gradient term ∇f by the stochastic gradient $\widehat{g}$ based on small batches

check out `torch.optim.SGD` at (their convention slightly differs from here)

https://pytorch.org/docs/stable/optim.html#torch.optim.SGD

Why SGD with adaptive learning rate?

Recall the struggle of GD on elongated functions, e.g., $f(x_1, x_2) = x_1^2 + 4x_2^2$



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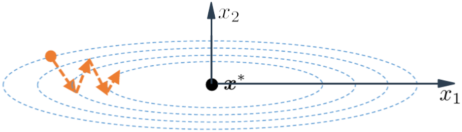

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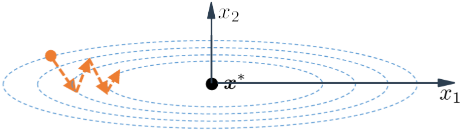

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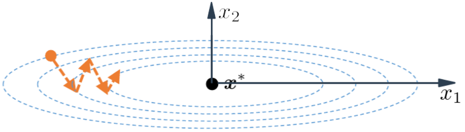

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Benefit: coordinate directions always with small (large) derivatives get sped up (slowed down). Think of the above $f(x_1, x_2)$ example!

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$$x_{i,k+1} = x_{i,k} - t_k \frac{g_{i,k}}{\sqrt{\sum_{j=1}^{k} g_{i,j}^2 + \varepsilon}}$$

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Typical values for β: $0.9, 0.99$. In PyTorch, `torch.optim.RMSprop`

https://pytorch.org/docs/stable/optim.html#torch.optim.RMSprop

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Combine RMSprop with momentum methods

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\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k - t_k \frac{\boldsymbol{m}_k}{\sqrt{\boldsymbol{s}_k + \varepsilon}}
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– Typical parameters: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\varepsilon =$ 1e-8.

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Combine RMSprop with momentum methods

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- In PyTorch, `torch.optim.Adam`
  https://pytorch.org/docs/stable/optim.html#torch.optim.Adam
- Several recent variants: `torch.optim.AdamW`, `torch.optim.SparseAdam`, `torch.optim.Adamax`

Thoughts on adaptive LR methods

– adapting the LR or adapting the (stochastic) gradient? Two views of the same thing ($\odot$ denotes elementwise product)

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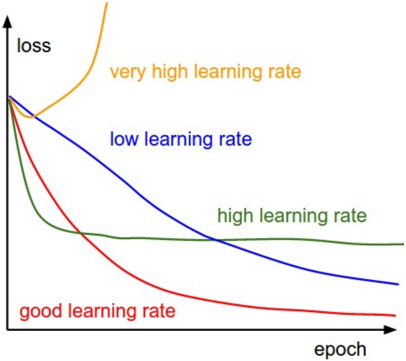
- Learning rate t_k: similar to that for the vanilla SGD, but less sensitive and can be large

Diagnosis of LR



Credit: Stanford CS231N

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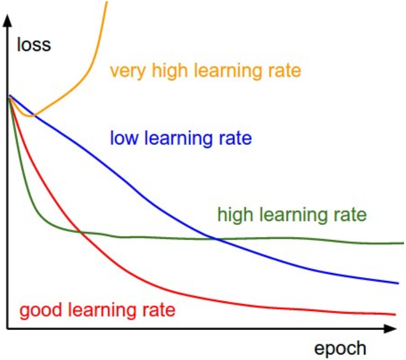

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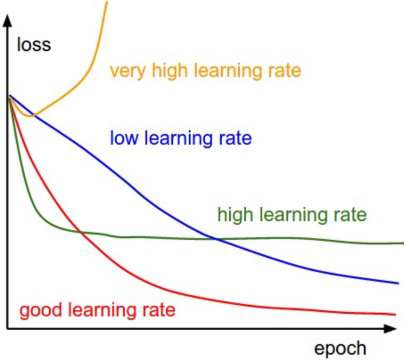

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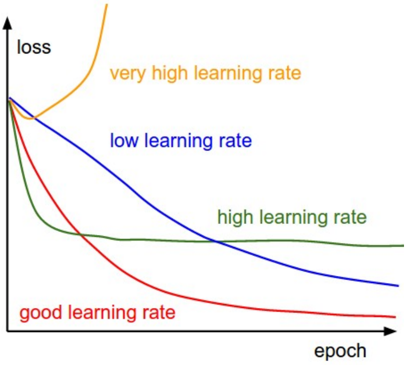

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- Remember the starecase LR schedule!

Why adaptive methods relevant for DL?

$$F\left(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_k\right) = \frac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \sigma\left(\boldsymbol{W}_k \sigma(\boldsymbol{W}_{k-1} \ldots (\boldsymbol{W}_1 \boldsymbol{x}_i))\right)\right)$$

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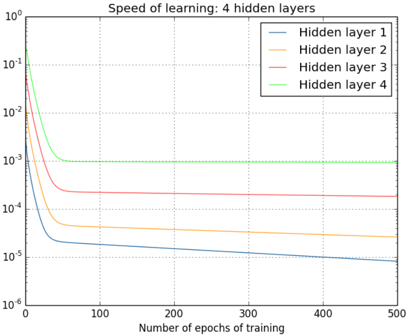

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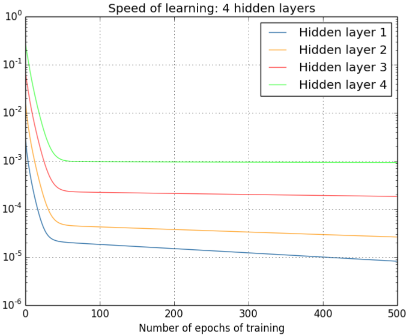

We'll explore more of this in HW3! See discussion in

http://neuralnetworksanddeeplearning.com/chap5.html

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- Adaptive methods can escape saddle points efficiently; see, e.g., [Staib et al., 2020]

visualization comparison https://imgur.com/a/Hqolp

Stochastic 2nd order methods

Recall scalable 2nd order methods

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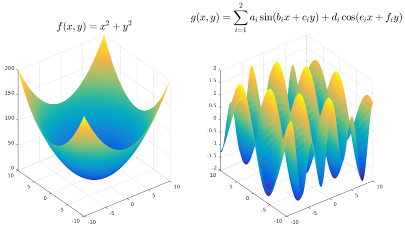
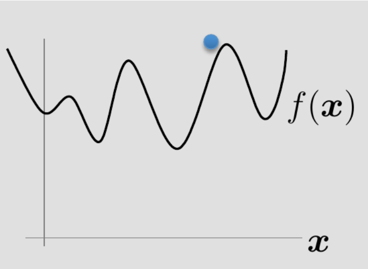
still active area of research. Hardware seems to be the main limiting factor

Outline

Where to initialize? the general picture



convex vs. nonconvex functions



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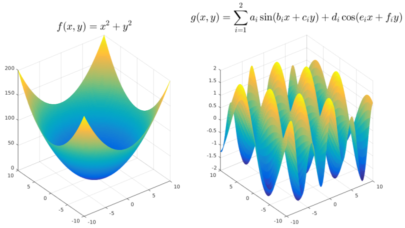

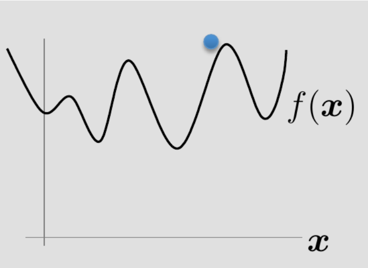

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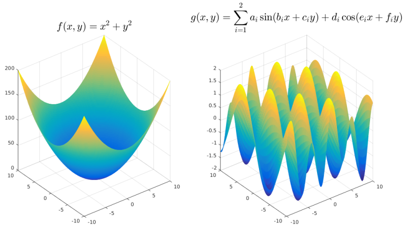

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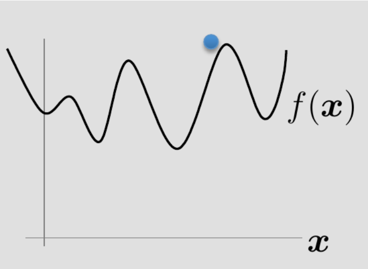

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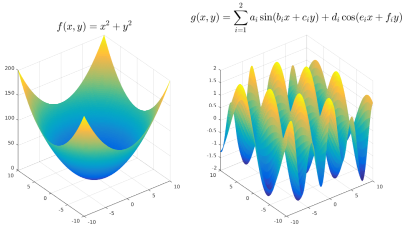

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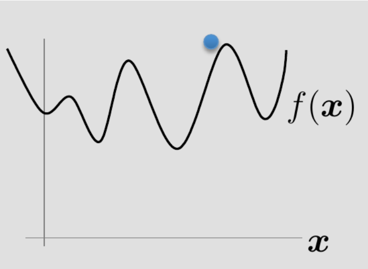

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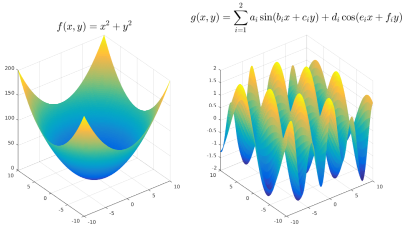

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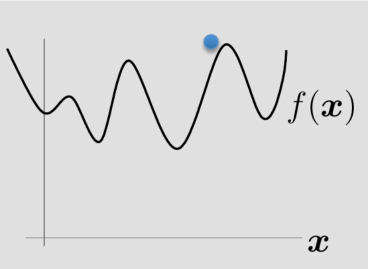

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https://sunju.org/research/nonconvex/

and sometimes random initialization works!

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  * random initialization with proper scaling
  * orthogonal initialization

Random initialization

Idea: make all entries in $\boldsymbol{W}$ iid random, and also $\boldsymbol{W}_i$'s and $\boldsymbol{W}_i^\intercal$'s "well behaved"

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A reasonable goal: if all entries in $\boldsymbol{v} \in \mathbb{R}^d$ are independent and have zero mean, unit variance, the output $\sigma\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right) \in \mathbb{R}$ (i.e., output of a single neuron) has a unit variance.

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For $\boldsymbol{W}_i$ with d inputs, set $\boldsymbol{W}_i$ iid zero-mean and $1/d$ variance

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For $\boldsymbol{W}_i$ with d_{in} inputs, set $\boldsymbol{W}_i$ iid zero-mean and $1/d_{\text{in}}$ variance

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- $\boldsymbol{W}_i \sim_{iid} \mathcal{N}\left(0, \frac{2}{d_{\text{in}}+d_{\text{out}}}\right)$ `torch.nn.init.xavier_normal_`
- $\boldsymbol{W}_i \sim_{iid} \text{uniform}\left(-\sqrt{\frac{6}{d_{\text{in}}+d_{\text{out}}}}, \sqrt{\frac{6}{d_{\text{in}}+d_{\text{out}}}}\right)$ `torch.nn.init.xavier_uniform_`

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Recall our derivation assumed σ is identity, which may not be accurate.

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For ReLU, based on the same assumptions on $\boldsymbol{v}$ and $\boldsymbol{w}$ as before:

$$
\begin{aligned}
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\operatorname{Var}\left(\operatorname{ReLU}\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right)\right) &= \mathbb{E}\left[\operatorname{ReLU}^2\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right)\right] = \frac{1}{2}\mathbb{E}\left[\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right)^2\right] \\
&= \frac{1}{2}\operatorname{Var}\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right) = \frac{1}{2} d \operatorname{Var}\left(w_i\right).
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$$\begin{aligned}\mathbb{E}\left[\mathrm{ReLU}\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right)\right] &= 0,\\ \mathrm{Var}\left(\mathrm{ReLU}\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right)\right) &= \mathbb{E}\left[\mathrm{ReLU}^2\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right)\right] = \frac{1}{2}\mathbb{E}\left[\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right)^2\right]\\ &= \frac{1}{2}\mathrm{Var}\left(\boldsymbol{w}^\intercal \boldsymbol{v}\right) = \frac{1}{2}d\mathrm{Var}\left(w_i\right).\end{aligned}$$

Kaiming Initialization (for ReLU): set $\boldsymbol{W}_i \in \mathbb{R}^{d_{\mathrm{out}} \times d_{\mathrm{in}}}$ iid zero-mean and $\frac{2}{d_{\mathrm{in}}}$-variance. For example:

Random initialization

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- $\boldsymbol{W}_i \sim_{iid} \mathcal{N}\left(0, \frac{2}{d_{\text{in}}}\right)$ `torch.nn.init.kaiming_normal_`
- $\boldsymbol{W}_i \sim_{iid} \mathrm{uniform}\left(-\sqrt{\frac{6}{d_{\text{in}}}}, \sqrt{\frac{6}{d_{\text{in}}}}\right)$ `torch.nn.init.kaiming_uniform_`

But it only accounts for d_{in} or d_{out}; a proposed modification: set the variance to $\frac{c}{\sqrt{d_{\text{in}} d_{\text{out}}}}$ for some constant c [Defazio and Bottou, 2019]

Orthogonal initialization

Making all $\boldsymbol{W}_i$'s orthonormal is empirically shown to lead to competitive performance with fewer tricks (covered next lectures). See Sec 4.2 of [Sun, 2019] `torch.nn.init.orthogonal_`

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There is a body of research proposing contraining/regularizing $\boldsymbol{W}_i$'s to be orthonormal, e.g., [Arjovsky et al., 2016, Bansal et al., 2018, Lezcano-Casado and Martínez-Rubio, 2019, Li et al., 2020]

See also the modified PyTorch package that allows manifold constraints

https://github.com/mctorch/mctorch

Outline

When to stop in training DNNs?

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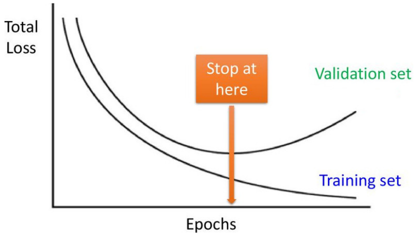
A practical/pragmatic stopping strategy: **early stopping**



... periodically check the validation error and stop when it doesn't improve

Outline

Suggested reading

- Sun, Ruoyu. "Optimization for deep learning: theory and algorithms." arXiv preprint arXiv:1912.08957 (2019).
- UIUC IE598-ODL Optimization Theory for Deep Learning https://wiki.illinois.edu/wiki/display/IE598ODLSP19/IE598-ODL++Optimization+Theory+for+Deep+Learning
- Stanford CS231n course notes: Neural Networks Part 1: Setting up the Architecture https://cs231n.github.io/neural-networks-1/
- Stanford CS231n course notes: Neural Networks Part 2: Setting up the Data and the Loss https://cs231n.github.io/neural-networks-2/
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[Li et al., 2020] Li, J., Fuxin, L., and Todorovic, S. (2020). **Efficient riemannian optimization on the stiefel manifold via the cayley transform.** *arXiv:2002.01113*.

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