Mathematics of Deep Learning

Non-convex optimization

Lessons: Kevin Scaman

Class overview

1.	Introduction and general overview	03/01
2.	**Non-convex optimization**	10/01
3.	Structure of ReLU networks and group invariances	17/01
4.	Approximation guarantees	24/01
5.	Stability and robustness	31/01
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7.	Generative models	14/02
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First-order optimization

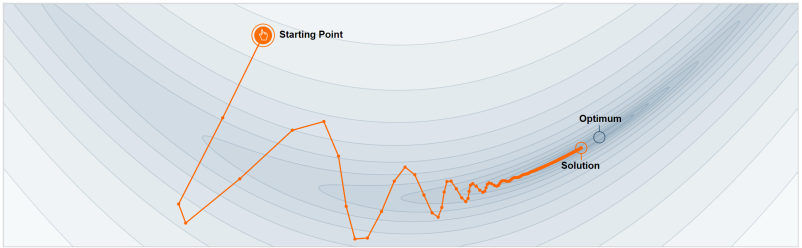
Gradient descent and co.

First-order optimization

- Find a **minimizer** $\theta^\star \in \mathbb{R}^d$ of a given objective function $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$,

$$\theta^\star \in \operatorname*{argmin}_{\theta \in \mathbb{R}^d} \mathcal{L}(\theta)$$

- Using an iterative algorithm relying on the **gradient** $\nabla \mathcal{L}(\theta_t)$ at each iteration $t \geqslant 0$.



source: https://distill.pub/2017/momentum/

First-order optimization

Iterative optimization algorithms

- **Initialization:** $\theta_0 \in \mathbb{R}^d$ (important in practice!).
- **Iteration:** Usually $\theta_{t+1} = \varphi_t\left(\theta_t, \nabla\mathcal{L}(\theta_t), s_t\right)$ where s_t is a hidden variable that is also updated at each iteration.
- **Stopping time:** $T > 0$ (also important in practice!).

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- **Non-convexity:** If $\mathcal{L}$ is **convex**, i.e. $\forall \theta, \theta', \mathcal{L}(\frac{\theta+\theta'}{2}) \leqslant \frac{\mathcal{L}(\theta)+\mathcal{L}(\theta')}{2}$, the optimization problem is **simple**. Most theoretical results use this assumption to prove convergence.

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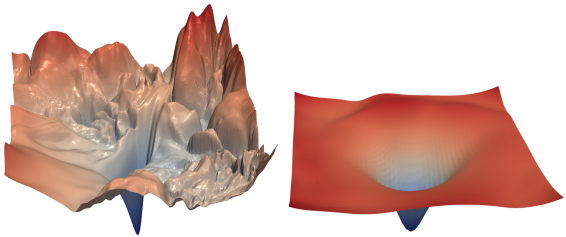
- **High dimensionality:** number of parameters $d \gg 1000$.
- **Access to the gradient:** the gradient of $\mathcal{L}$ is too expensive to compute! In practice, $\nabla\mathcal{L}(\theta_t)$ is replaced by a **stochastic** or **mini-batch** approximation $\widetilde{\nabla}_t$.

Loss landscape

Training a neural network requires solving a difficult non-convex optimization problem

$$\min_{\theta \in \mathbb{R}^d} \frac{1}{N} \sum_{i=1}^{N} \ell\left(g_\theta(x_i), y_i\right)$$

Ex: loss landscape around the optimum for ResNet-56 trained on CIFAR10.



(a) without skip connections (b) with skip connections

source: Visualizing the Loss Landscape of Neural Nets. Li et.al., 2018.

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In general, the regularity of the objective will depend on the architecture of the neural network, and part of DL research is devoted to finding architecture that are easy to train.

Ideal optimization theory for DL training

- Should provide **fast gradient computation** for composition of modules.
- Should explain performances of **non-convex SGD** (and its variants).
- Should work in **high-dimensional** spaces.
- Should extend to **non-smooth** objectives.
- Should have assumptions that are **reasonable for neural networks**.

Next steps

1. Understand how the **gradient is computed** in Pytorch.
2. Understand why **stochastic gradient works**.

Some warnings about optimization in deep learning

Our final goal is to reduce the **population risk**, i.e. $\mathbb{E}(\ell(g_\theta(X), Y))$!

- We need to pay attention to **overfitting** in addition to using the optimization algorithm to reduce the training error.
- In this class, we focus specifically on the **performance** of the optimization algorithm in minimizing the objective function, rather than the model's generalization error.
- In the next lessons, we will see techniques to avoid **overfitting**.

Automatic differentiation

A short recap on differentiating composite functions

Existing approaches to compute gradients

- **Finite differences:** small perturbations $g'(x) \approx \frac{g(x+\varepsilon)-g(x)}{\varepsilon}$. Leads to **round-off** errors.

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Chain rule (simple version)

Let $f, g : \mathbb{R} \to \mathbb{R}$ differentiable, then

$$(f \circ g)' = (f' \circ g) \cdot g'$$

Recap: derivatives of multi-dimensional functions

Definition (Jacobian matrix)

Let $f : \mathbb{R}^n \to \mathbb{R}^m$ a differentiable function. Its Jacobian $J_f(x) \in \mathbb{R}^{m \times n}$ is the matrix whose coordinates are the partial derivatives:

$$J_f(x) = \begin{bmatrix} \nabla f_1(x)^\top \\ \cdots \\ \nabla f_m(x)^\top \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_1} & \cdots & \frac{\partial f_1(x)}{\partial x_n} \\ \cdots & \cdots & \cdots \\ \frac{\partial f_m(x)}{\partial x_1} & \cdots & \frac{\partial f_m(x)}{\partial x_n} \end{bmatrix}$$

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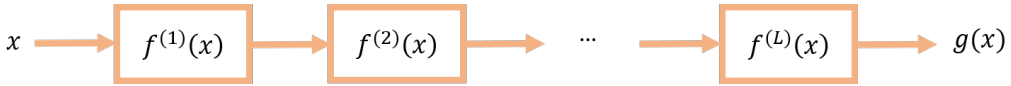
Chain rule (multi-dimensional version)

Let $f : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^p \to \mathbb{R}^n$ differentiable, then

$$J_{f \circ g} = (J_f \circ g) \times J_g$$

Derivative of a composition of functions



Composite function

- Let $f^{(l)} : \mathbb{R}^{d^{(l-1)}} \to \mathbb{R}^{d^{(l)}}$ and $g(x) = g^{(L)}(x)$ where

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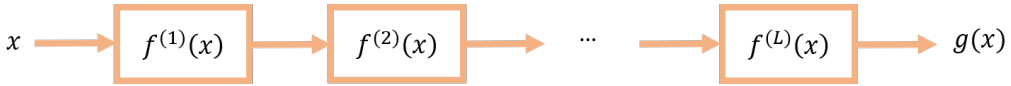

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- Then, the Jacobian matrix (i.e. matrix of derivatives) of g is

$$J_g(x) = J_{f^{(L)}}\left(g^{(L-1)}(x)\right) \times \cdots \times J_{f^{(2)}}\left(g^{(1)}(x)\right) \times J_{f^{(1)}}(x)$$

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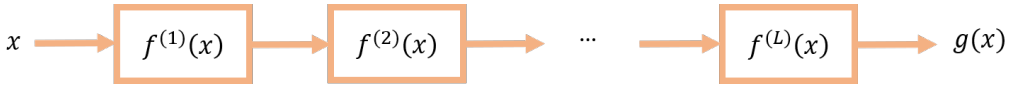

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- What is the **computational complexity** to compute the Jacobian matrix?

Computational complexity

Finite differences

- The gradient of g can be approximated by **finite differences**: $\nabla g(x)_i \approx \frac{g(x+\varepsilon e_i)-g(x)}{\varepsilon}$
- **Computational complexity:** proportional to **input dimension**.

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- **Backward propagation:** Compute $\nabla g(x)^\top = (((J_L \times J_{L-1}) \times \cdots \times J_2) \times J_1)$. If output is 1-dimensional, only needs **matrix-vector products**!

Which algorithm is faster?

Complexity for gradients of MLPs

- Let $g_\theta : \mathbb{R}^d \to \mathbb{R}$ an MLP of width $w \geqslant d$ and depth $L \geqslant 1$.
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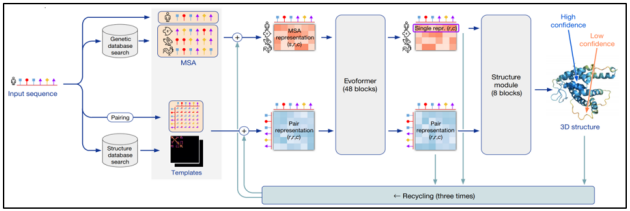
Intuition for gradients w.r.t. parameters

- Finite differences requires **two function calls per parameter**.
- Backprop requires **O(1) function calls for the whole gradient**.
- Interpretation as parameter testing:
  - Each partial derivative w.r.t. a parameter indicates if this parameter can describe the data.
  - With backprop, we can test **all parameters at once**.

Computation graphs: intuition

Complex neural network architecture (e.g. AlphaFold)



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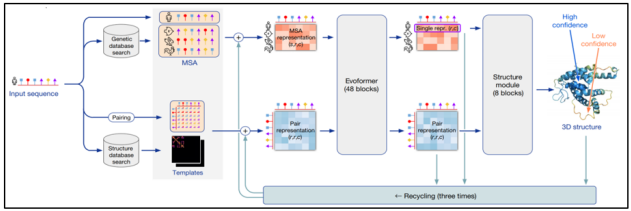

Code (e.g. Python)

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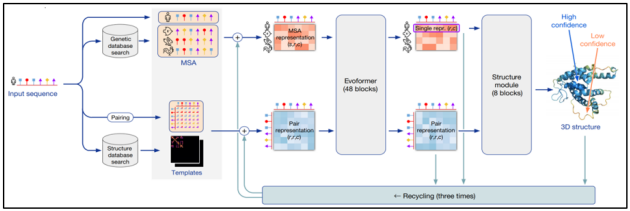

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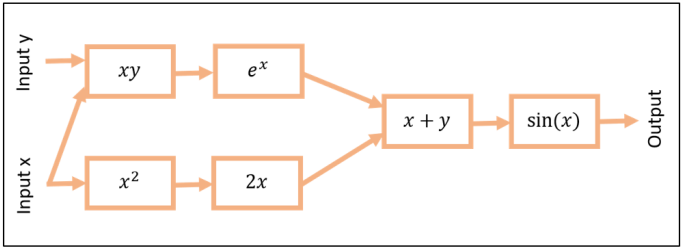
Computation graph (DAG of mathematical operations)



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- **Chain rule:** partial gradient $\frac{\partial x^{(f)}}{\partial x^{(v)}}$ for a node $v \in V$ from that of its children.

$$\frac{\partial x^{(f)}}{\partial x^{(v)}} = \sum_{w \in \mathsf{Children}(v)} \frac{\partial f^{(w)}\left((x^{(w')})_{w' \in \mathsf{Parents}(w)}\right)}{\partial x^{(v)}}^{\top} \frac{\partial x^{(f)}}{\partial x^{(w)}}$$

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- **BP:** Let $z^{(f)} = 1$ and, for $v \in V/F$, we compute iteratively **from leaf to roots**,

$$z^{(v)} = \sum_{w \in \mathsf{Children}(v)} \frac{\partial f^{(w)}\left((y^{(w')})_{w' \in \mathsf{Parents}(w)}\right)}{\partial x^{(v)}}^{\top} z^{(w)}$$

- Then, for all $r \in R$, we have $\frac{\partial \mathcal{L}(\theta)}{\partial \theta^{(r)}} = z^{(r)}$.

Non-convex optimization

Convergence to local/global minima

Optimizing non-convex functions is hard...

Assumptions

- The objective function is **non-convex**, **differentiable** and β-**smooth**, i.e. $\forall \theta, \theta' \in \mathbb{R}^d$,

$$\|\nabla \mathcal{L}(\theta) - \nabla \mathcal{L}(\theta')\|_2 \leqslant \beta \|\theta - \theta'\|_2$$

- We access unbiased noisy gradients $\widetilde{\nabla}_t$ where $\mathbb{E}(\widetilde{\nabla}_t) = \nabla \mathcal{L}(\theta_t)$ and $\mathrm{var}(\widetilde{\nabla}_t) \leqslant \sigma^2$.

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Proposition (worst-case convergence to global optimum)

For any first-order algorithm, there exists a smooth function $\mathcal{L}$ such that approx. error is at least

$$\mathcal{L}(\theta_t) - \mathcal{L}(\theta^\star) = \Omega(t^{-2/d})$$

This is prohibitive for large dimensional spaces (i.e. $d \geqslant 100$)!

Convergence of SGD... to a stationary point

Theorem (convergence of non-convex SGD)

Let $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$ be a smooth function and $\Delta = \mathcal{L}(\theta_0) - \mathcal{L}(\theta^\star)$. Then, SGD with step-size $\eta \leqslant \frac{1}{\beta}$ achieves the error

$$\mathbb{E}\big[\min_{t \leqslant T} \|\nabla \mathcal{L}(\theta_t)\|^2\big] \leqslant \frac{2\Delta}{\eta T} + \beta \eta \sigma^2$$

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- Convergence only possible for **decreasing step-sizes**, with optimal cv. in $O(1/\sqrt{T})$.

Convergence to a local minimum

How to obtain local minimum?

- A local minimum can be defined using second order derivatives:
  1. **Stationarity:** $\nabla \mathcal{L}(\theta) = 0$
  2. **Convexity:** the Hessian $H_{\mathcal{L}}(x)$ is SDP.

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Convergence to a local minimum (Jin et.al., 2017)

- Adding a small noise allows the parameter to escape saddle points.
- Additional assumption: the Hessian $H_{\mathcal{L}}$ is ρ-Lipschitz w.r.t. spectral norm.
- With probability at least $1 - \delta$, the number of iterations to reach a gradient norm $\|\nabla \mathcal{L}(\theta_t)\| \leqslant \varepsilon$ and near-convexity $\lambda_1(H_{\mathcal{L}}(\theta_t)) \geqslant -\sqrt{\rho\varepsilon}$ is bounded by

$$O\left(\frac{\beta\Delta}{\varepsilon^2}\log\left(\frac{d\beta\Delta}{\varepsilon\delta}\right)^4\right)$$

Recap

- The loss landscape of DL training is **non-convex** and potentially difficult to optimize.
- Convergence to a **global minimum prohibitive** in high-dimensional spaces.
- GD converges to a **stationary point** with constant step-sizes.
- SGD converges (more slowly) to a **stationary point** with decreasing step-sizes.
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- Adding noise is necessary to converge to a **local minimum** (Jin et.al., 2017).
- We need **stronger assumptions** on the objective function to go beyond...

Beyond local minimisation

The Łojasiewicz condition

A look at the proof of convergence of SGD

- By smoothness, we have, for $\theta_{t+1} = \theta_t - \eta G_t$,

$$\mathbb{E}(\mathcal{L}(\theta_{t+1})) - \mathbb{E}(\mathcal{L}(\theta_t)) \leqslant -\eta \left(1 - \frac{\beta\eta}{2}\right) \mathbb{E}(\|\nabla \mathcal{L}(\theta_t)\|^2) + \frac{\beta\eta^2\sigma^2}{2}$$

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- When $\mathcal{L}$ is α-strongly convex, we have $\|\nabla \mathcal{L}(\theta_t)\|^2 \geqslant 2\alpha(\mathcal{L}(\theta_t) - \mathcal{L}(\theta^\star))$.
- If $\eta \leqslant 1/\beta$, this implies, for $\varepsilon_t = \mathbb{E}(\mathcal{L}(\theta_t)) - \mathbb{E}(\mathcal{L}(\theta^\star))$,

$$\varepsilon_{t+1} \leqslant (1 - \alpha\eta)\, \varepsilon_t + \frac{\beta\eta^2\sigma^2}{2}$$

The Polyak-Łojasiewicz condition

Definition (Polyak & Łojasiewicz, 1963)

A function $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$ is said to verify the μ-Polyak-Łojasiewicz (PL) condition iff

$$\|\nabla \mathcal{L}(\theta_t)\|^2 \geqslant 2\mu \left(\mathcal{L}(\theta_t) - \mathcal{L}(\theta^\star)\right)$$

where $\theta^\star \in \mathbb{R}^d$ is a global minimum of the function $\mathcal{L}$ and $\mu > 0$ is a constant.

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Theorem (convergence of SGD under μ-PL)

If $\mathcal{L}$ is β-smooth and verifies the PL condition, then, with $\eta \leqslant \frac{1}{\beta}$, SGD achieves the precision

$$\mathbb{E}(\mathcal{L}(\theta_T) - \mathcal{L}(\theta^\star)) \leqslant \Delta \left(1 - \mu\eta\right)^T + \frac{\beta\eta\sigma^2}{2\mu}$$

Exponential convergence rate $O(e^{-T})$ without noise, and $O(\ln(T)/T)$ otherwise.

Beyond strongly convex functions

Is the PL condition satisfied for more than strongly-convex functions?

Examples

- For $\mathcal{L}(\theta) = (\theta_1 - \cos(\theta_2))^2$, we have $\|\nabla \mathcal{L}(\theta)\|^2 =$

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Examples

- For $\mathcal{L}(\theta) = (\theta_1 - \cos(\theta_2))^2$, we have $\|\nabla \mathcal{L}(\theta)\|^2 = 4\mathcal{L}(\theta)(1 + \sin(\theta_2)^2) \geqslant 4\mathcal{L}(\theta)$.

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- More gl. if $\mathcal{L}(\theta) = g(\theta)^2$ and $\|\nabla g(\theta)\| \geqslant c$ for any $\theta \in \mathbb{R}^d$, then $\|\nabla \mathcal{L}(\theta)\|^2 \geqslant 4c^2 \mathcal{L}(\theta)$.

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Theorem (PL condition for compositions)

Let $\mathcal{L}(\theta) = (f \circ g)(\theta)$ where f satisfies the μ-PL condition and g is such that, $\forall \theta \in \mathbb{R}^d$

$$\sigma_{\min}\left(J_g(\theta)^\top\right) \geqslant \varepsilon\,,$$

where $\sigma_{\min}(M) = \min_{x \neq 0} \|Mx\|/\|x\|$ is the smallest singular value of the matrix M. Then $\mathcal{L}$ verifies the μ'-PL condition with $\mu' = \mu\varepsilon^2$.

PL for neural networks

Theorem (PL condition for MSE loss)

Let $\mathcal{L}(\theta) = \frac{1}{N}\sum_{i=1}^{N} \ell(g_\theta(x_i), y_i)$ where $\ell(y, y') = \|y - y'\|_2^2$ and the model g_θ is such that

$$\sigma_{\min}\left(\left(J_{g,\theta}(x_1,\theta)^\top \;\middle|\; \cdots \;\middle|\; J_{g,\theta}(x_N,\theta)^\top\right)\right) \geqslant \varepsilon$$

then $\mathcal{L}$ verifies the μ-PL condition with $\mu = 4\varepsilon^2/N$.

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then $\mathcal{L}$ verifies the μ-PL condition with $\mu = 4\varepsilon^2/N$.

- For **over-parameterized neural networks**, this quantity is usually controlled for $\theta = \theta_0$ (if the weights are **properly initialized**, see lesson 5), and valid on a neighborhood around initialization (linked with the **Neural Tangent Kernel**, see lesson 6). For example, **uniform conditioning** (Liu et al., 2020) assumes that the singular value is lower bounded for all $\theta \in \mathcal{B}(\theta_0, R)$.

Recap

- The loss lanscape of DL training is **non-convex** and potentially difficult to optimize.
- Convergence to a global minimum for any smooth function is **prohibitive in high-dimensional spaces** (exponential in $d/2$).
- SGD ($+$ noise) can converge, within an error $\varepsilon > 0$, to a **local minimum** of any smooth function in roughly $O(\varepsilon^{-2})$ iterations.
- By relaxing the convexity constraint to a **PL condition**, one can obtain **convergence to the global optimum**.
- The PL condition is verified for neural networks whose **singular values of the Jacobian are bounded from below**.