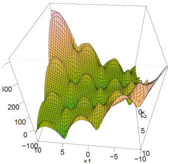
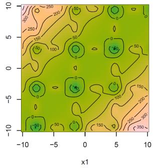
Optimization in Machine Learning

First order methods
GD – Multimodality and Saddle points

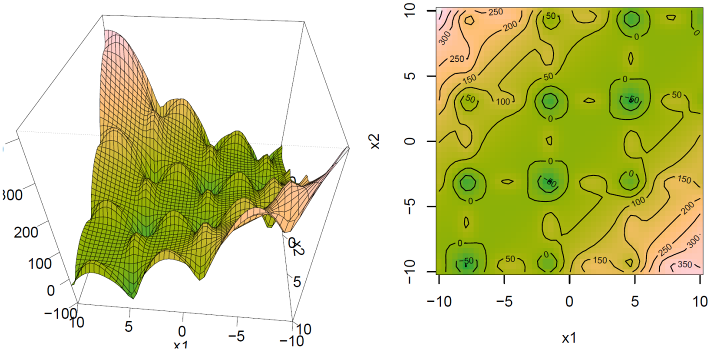




Learning goals

- Multimodality, GD result can be arbitrarily bad
- Saddle points, major problem in NN error landscapes, GD can get stuck or slow crawling

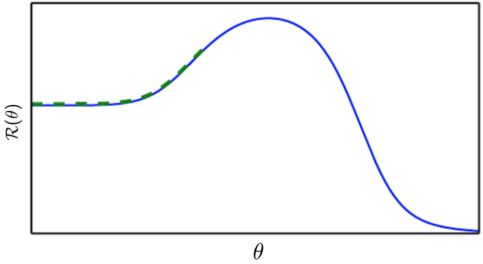
UNIMODAL VS. MULTIMODAL LOSS SURFACES



Snippet of a loss surface with many local optima

GD: ONLY LOCALLY OPTIMAL MOVES

- GD makes only **locally** optimal moves
- It may move away from the global optimum

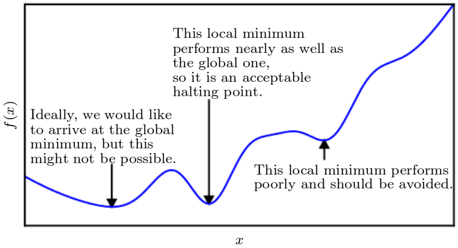


Source: Goodfellow et al., 2016

- Initialization on “wrong” side of the hill results in weak performance
- In higher dimensions, GD may move around the hill (potentially at the cost of longer trajectory and time to convergence)

LOCAL MINIMA

- **In practice:** Only local minima with high value compared to global minimium are problematic.



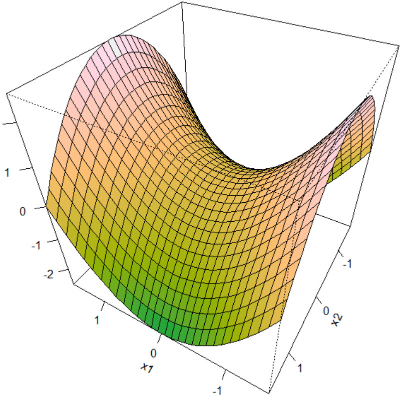
Source: Goodfellow et al., 2016

GD AT SADDLE POINTS

Example:

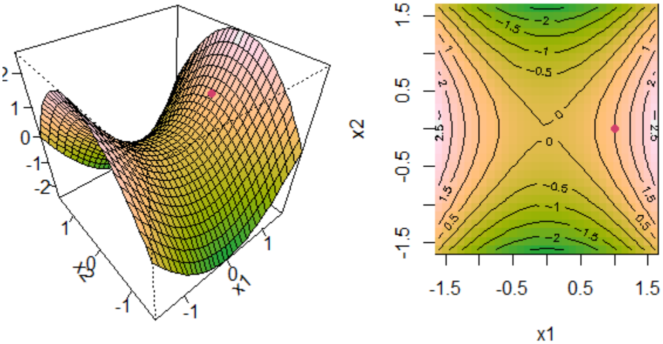
$$
\begin{aligned}
f(x_1, x_2) &= x_1^2 - x_2^2 \\
\nabla f(x_1, x_2) &= (2x_1, -2x_2)^\top \\
\boldsymbol{H} &= \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}
\end{aligned}
$$

- Along x_1, curvature is positive ($\lambda_1 = 2 > 0$).
- Along x_2, curvature is negative ($\lambda_2 = -2 < 0$).



EXAMPLE: SADDLE POINT WITH GD

- How do saddle points impair optimization?
- Gradient-based algorithms **might** get stuck in saddle points



Red dot: Starting location

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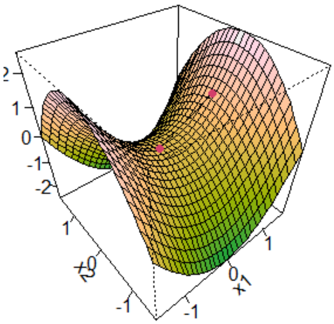

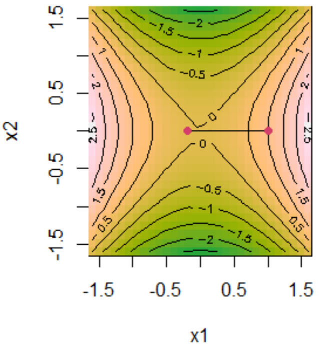

Step 1 ...

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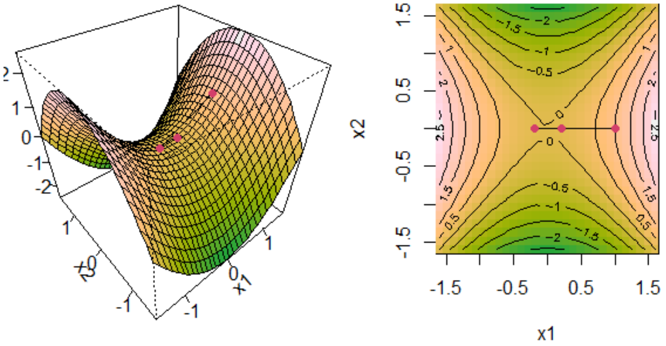

... Step 2 ...

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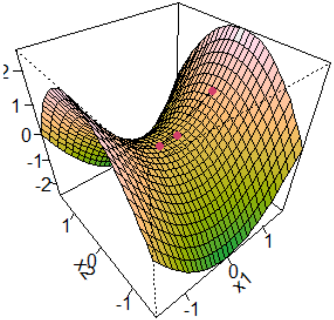

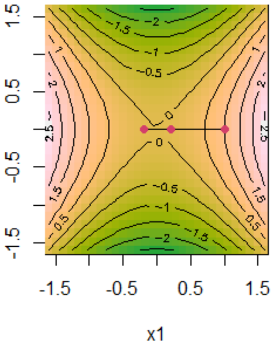

... Step 10 ... got stuck and cannot escape saddle point

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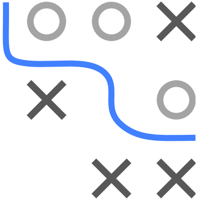

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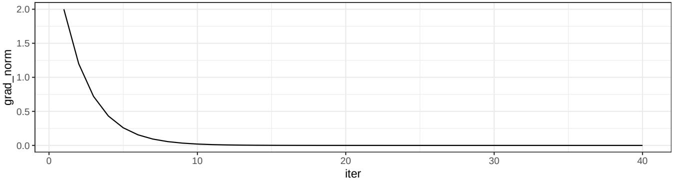

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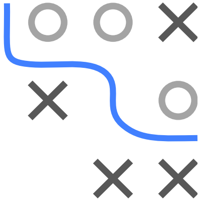
SADDLE POINTS IN NEURAL NETWORKS



- For the empirical risk $\mathcal{R} : \mathbb{R}^d \rightarrow \mathbb{R}$ of a neural network, the expected ratio of the number of saddle points to local minima typically grows exponentially with d
- In other words: Networks with more parameters (deeper networks or larger layers) exhibit a lot more saddle points than local minima
- **Reason:** Hessian at local minimum has only positive eigenvalues. Hessian at saddle point has positive and negative eigenvalues.