NYU CS-GY 6923 Machine Learning

Prof. Pavel Izmailov

Guest lecturer: Timur Garipov

Introduction

Timur Garipov

- Collaborating with Pavel since 2016
- PhD, MIT CSAIL, 2024
- Now AI research in industry

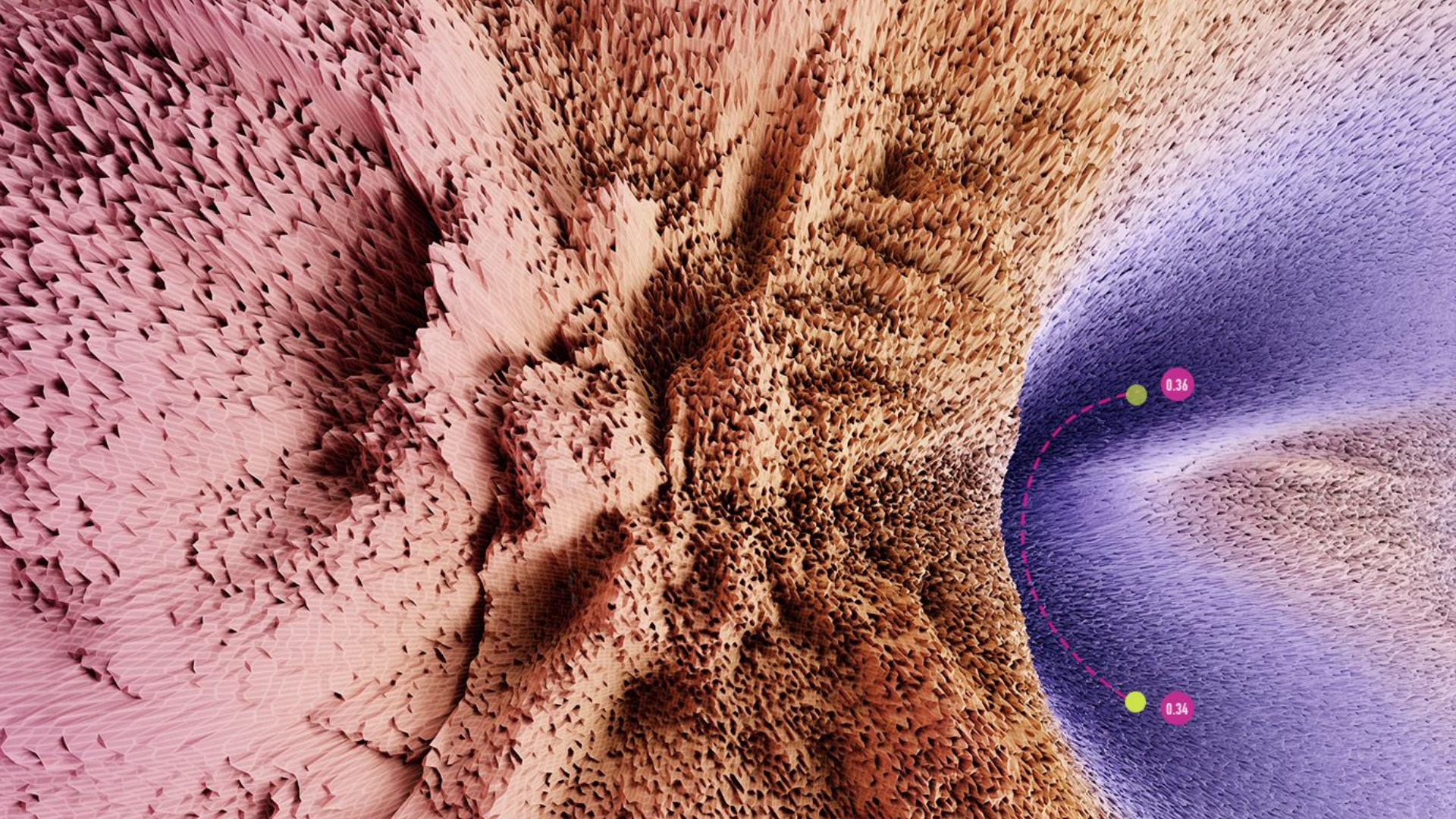
Research Interests

- Deep Learning
- Deep Probabilistic Models / Generative Models
- LLM reasoning

Today

Optimization in Machine Learning

- (Regularized) Empirical Risk Minimization
- Gradient Descent & Stochastic Gradient Descent
- Theoretical and Practical Aspects
- Non-convex loss landscapes: Deep Neural Networks
- Beyond optimization:
  - Game-theoretic formulations
  - Dynamical systems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Machine Learning

Given: training data

Want: predictive model f(x)

Such that:

- Model “agrees” with observed data
- Model provides useful predictions for previously unobserved inputs

Learning Algorithm:

Training Data => [Algorithm] => Model

Learning Algorithm

Learning Algorithm:

Training Data => [Algorithm] => Model

How do we design and analyse a learning algorithm?

Empirical Risk Minimization

- Model “agrees” with observed data
- Model provides useful predictions for previously unobserved inputs

Empirical Risk Minimization:

- Pick a model family (e.g. linear models / neural networks / …)
- Find a model that minimizes error on training data

$$\min_{\texttt{model}} \quad \sum_{i=1}^{N} \ell(x_i, y_i, \texttt{model}) \;+\; \lambda \cdot R(\texttt{model})$$

$\texttt{model} \in$ Model Family

Empirical Risk Minimization

Why ERM?

$$\min_{\texttt{model}} \sum_{i=1}^{N} \ell(x_i, y_i, \texttt{model}) + \lambda \cdot R(\texttt{model})$$

$\texttt{model} \in$ Model Family

Assume $(x_i, y_i) \overset{iid}{\sim} P(x, y)$

Empirical error : $\hat{\mathcal{L}}(\texttt{model}) = \sum_{i=1}^{N} \ell(x_i, y_i, \texttt{model})$

Population error : $\mathcal{L}(\texttt{model}) = \mathbb{E}_{P(x,y)}\left[\ell(x, y, \texttt{model})\right]$

In-distribution generalization: test data comes from the same distribution

Recap: Linear Regression; Logistic Regression

Linear regression:

$$\min_{w,w_0} \sum_{i=1}^{N} \left(\langle w, x_i \rangle + w_0 - y_i\right)^2 + \lambda \cdot \|w\|^2$$

Logistic regression:

$$\min_{w,w_0} \sum_{i=1}^{N} \log\left(1 + \exp\left(-y_i(\langle w, x_i \rangle + w_0)\right)\right) + \lambda \cdot \|w\|^2$$

Recap: Linear Regression; Logistic Regression

Linear regression:

$$\min_{w,w_0} \sum_{i=1}^{N} \left(\langle w, x_i \rangle + w_0 - y_i\right)^2 + \lambda \cdot \|w\|^2$$

Maximum Likelihood Estimate (MLE):

$$\min_{w,w_0} \sum_{i=1}^{N} -\log p(y_i \mid x_i, w, w_0)$$

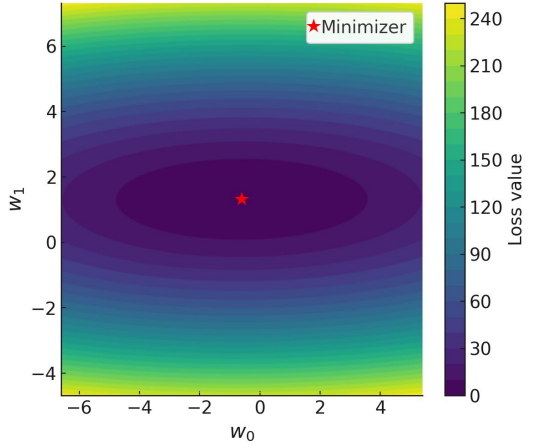
Maximum a Posteriori Estimate(MAE):

$$\min_{w,w_0} \sum_{i=1}^{N} -\log p(y_i \mid x_i, w, w_0) - \log p(w, w_0)$$

Recap: Linear Regression; Logistic Regression

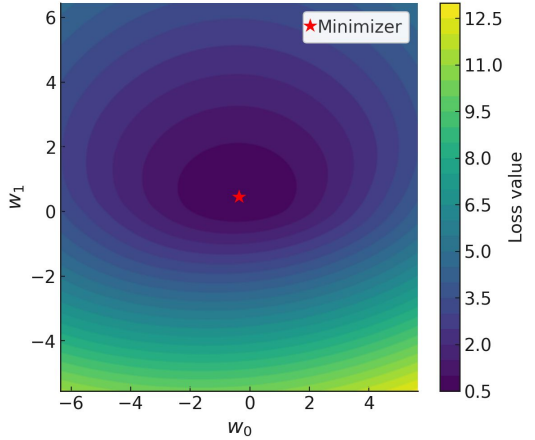
Linear regression:

- Loss function is a quadratic function of w
- Has analytical expression for the optimal solution
- Requires costly inversion of DxD matrix



Logistic regression:

- Loss function involves log(1 + exp(f(x, y, w))
- No analytical expression for the optimal solution
- Requires an optimization algorithm



Today

ML via optimization. Find “good” model by

- Minimizing Empirical Risk (Maximizing Likelihood)

Optimization questions:

- Model parameterization + error function → **loss landscape** properties?
- Does the **optimization algorithm** converge to a minimizer?
- What is algorithm’s **convergence rate**?

Machine learning questions:

- **Generalization**: Does the **optimal solution** have useful statistical properties?
- How much **regularization** do we need?
- **Implicit regularization:** Do we want to solve optimization “precisely”?

Optimization

Logistic regression: $$\min_w \sum_{i=1}^{N} \log\left(1 + \exp\left(-y_i \langle w, x_i \rangle\right)\right) + \lambda \cdot \|w\|^2$$

$\min_{w \in \mathbb{R}^d} f(w)$ — unconstrained optimization problem in $\mathbb{R}^d$

“Hardness” of the problem depends on:

- Mathematical properties of the function (smoothness, convexity)
- Number of dimensions
- Computational cost of evaluating f, its gradients, Hessians, …

For general non-convex functions the problem is NP-hard

Gradient Descent

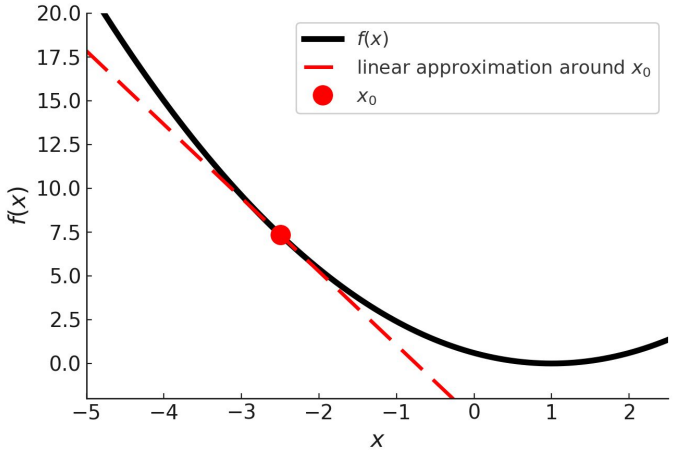
$$\min_{w \in \mathbb{R}^d} f(w)$$ — unconstrained optimization problem in $\mathbb{R}^d$

If f is smooth, then

$$f(x_0 + h) = f(x_0) + \langle \nabla_x f(x_0), h \rangle + O(\|h\|^2)$$

The direction of the fastest descent is

$$h = -\nabla_x f(x_0)$$



Let's take a step in that direction!

Gradient Descent

$$\min_{w \in \mathbb{R}^d} f(w)$$ — unconstrained optimization problem in $\mathbb{R}^d$

Gradient descent

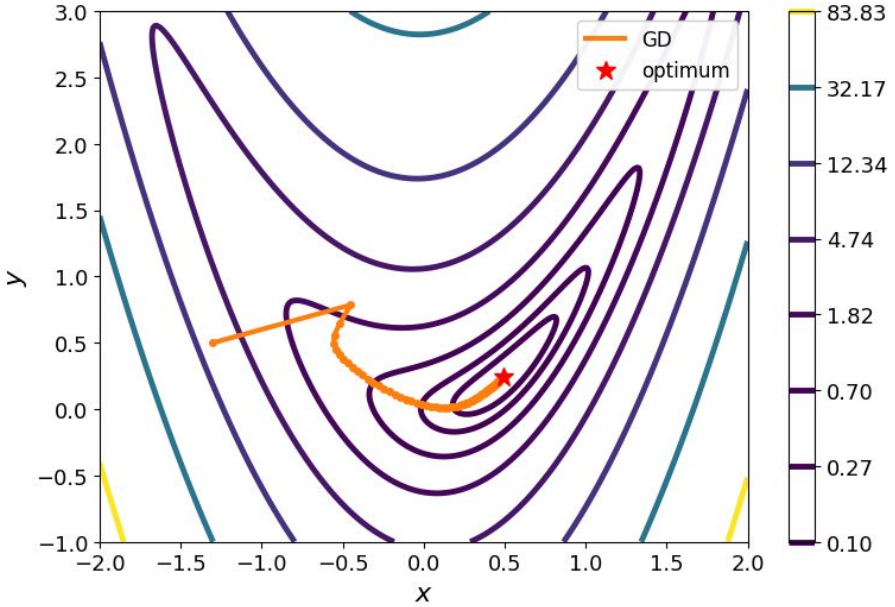
Pick x_0; set $k = 0$

Until `should_stop()` :

$$x_{k+1} = x_k - \alpha_k \cdot \nabla_x f(x_k)$$
$$k = k + 1$$

Algorithm parameters:

- Step-size schedule
- Stopping criterion



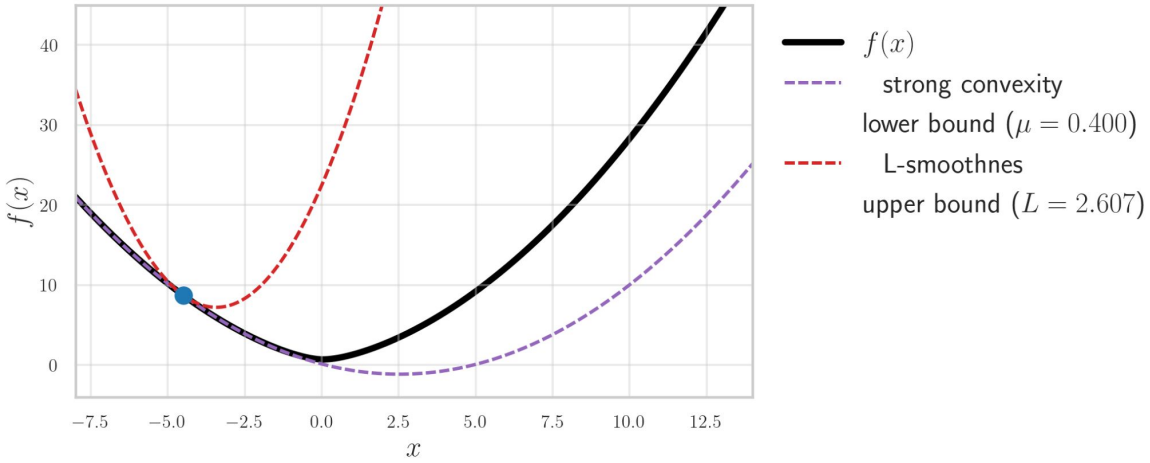
Gradient Descent: Convergence

Assume $f : \mathbb{R}^d \to \mathbb{R}$ is μ-strongly convex and L-smooth, and let $x^\star = \arg\min f$.

Strong convexity: $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2}\|y - x\|^2, \quad \forall\, x, y.$

L-smooth (L-Lipshitz gradient): $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|, \quad \forall\, x, y.$

Consequence (Descent Lemma): $f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2}\|y - x\|^2, \quad \forall\, x, y.$



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Gradient descent with step size $\alpha_k = \frac{1}{L} \quad x_{k+1} = x_k - \frac{1}{L}\nabla f(x_k).$

Linear convergence: $f(x_k) - f(x^\star) \leq \left(1 - \frac{\mu}{L}\right)^k \left(f(x_0) - f(x^\star)\right).$

$k(\varepsilon)$ such that $f(\bar{x}_k) - f(x^\star) \leq \varepsilon \Leftarrow k(\varepsilon) = O\left(\log \frac{1}{\varepsilon}\right)$

Gradient Descent: Convergence (Proof I)

L-smooth (L-Lipshitz gradient): $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|, \quad \forall\, x, y.$

Consequence (Descent Lemma): $f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2}\|y - x\|^2, \quad \forall\, x, y.$

Gradient descent with step size $\alpha_k = \frac{1}{L} \quad x_{k+1} = x_k - \frac{1}{L}\nabla f(x_k).$

Apply descent lemma with $x = x_k, ; y = x_{k+1}$:

$$\begin{aligned} f(x_{k+1}) &\leq f(x_k) + \left\langle \nabla f(x_k), -\frac{1}{L}\nabla f(x_k) \right\rangle + \frac{L}{2}\left\| - \tfrac{1}{L}\nabla f(x_k) \right\|^2 \\ &= f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2. \end{aligned}$$

Gradient Descent: Convergence (Proof II)

Strong convexity: $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2}\|y - x\|^2, \quad \forall\, x, y.$

Strong convexity $\Rightarrow$ lower bound on gradient norm

$$f(x^\star) \geq f(x) + \langle \nabla f(x), x^\star - x \rangle + \frac{\mu}{2}\|x^\star - x\|^2$$

$$\Rightarrow f(x) - f(x^\star) \leq \langle \nabla f(x), x - x^\star \rangle - \frac{\mu}{2}\|x - x^\star\|^2$$

$$\leq \|\nabla f(x)\|\,\|x - x^\star\| - \frac{\mu}{2}\|x - x^\star\|^2$$

Consider quadratic in $t = \|x - x^\star\|$: $\quad \|\nabla f(x)\|\, t - \frac{\mu}{2}t^2 \leq \max_{t \geq 0}\left(\|\nabla f(x)\|\, t - \frac{\mu}{2}t^2\right)$

Maximum occurs at $t = \dfrac{\|\nabla f(x)\|}{\mu}$, giving value $\dfrac{1}{2\mu}\|\nabla f(x)\|^2$

$$f(x) - f(x^\star) \leq \frac{1}{2\mu}\|\nabla f(x)\|^2 \quad \Rightarrow \quad \|\nabla f(x)\|^2 \geq 2\mu\big(f(x) - f(x^\star)\big).$$

Gradient Descent: Convergence (Proof III)

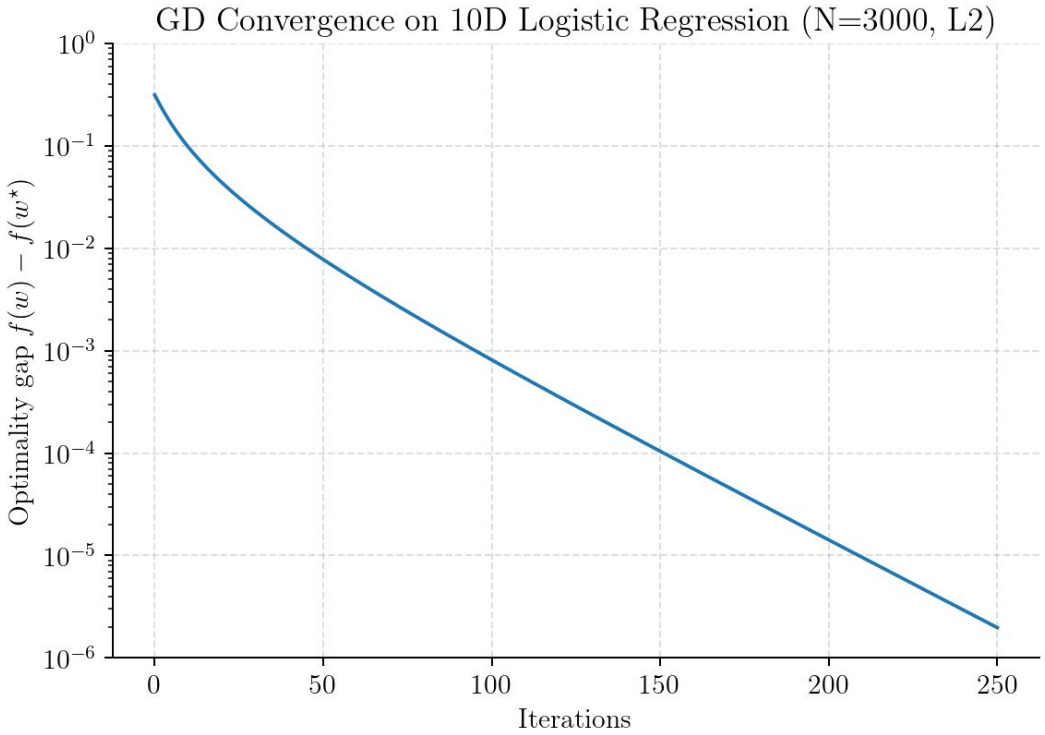
$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2. \qquad \|\nabla f(x)\|^2 \geq 2\mu\big(f(x) - f(x^\star)\big).$$

Combine bounds:

$$\begin{aligned} f(x_{k+1}) - f(x^\star) &\leq f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2 - f(x^\star) \\ &\leq f(x_k) - f(x^\star) - \frac{\mu}{L}\big(f(x_k) - f(x^\star)\big) \\ &= \Big(1 - \frac{\mu}{L}\Big)\big(f(x_k) - f(x^\star)\big). \end{aligned}$$

Linear convergence: $f(x_k) - f(x^\star) \leq \Big(1 - \frac{\mu}{L}\Big)^k \big(f(x_0) - f(x^\star)\big).$

Gradient Descent: Convergence. Example



Gradient Descent: Evaluation Cost

$$f(w) = \frac{1}{N}\sum_{i=1}^{N} \log\left(1 + \exp(-y_i \cdot \langle w, x_i \rangle\right) + \lambda \cdot \|w\|^2$$

$$= \frac{1}{N}\sum_{i=1}^{N} f_i(w) + R(w)$$

$$\nabla_w f(w) = \frac{1}{N}\sum_{i=1}^{N} \nabla_w f_i(w) + \nabla_w R(w)$$

One gradient descent step requires accumulating gradient over the entire dataset

How do we handle large datasets?

Well, large dataset is just many small datasets :-)

Full gradient → batch gradient

Batch: $B_m = [i_1, \ldots, i_m]$

- collection of m indices, $m \ll N$
- randomly selected (e.g. uniformly with replacement).

$$f(w) = \frac{1}{N} \sum_{i=1}^{N} f_i(w) + R(w)$$

Batch loss

$$f_{B_m}(w) = \frac{1}{m} \sum_{i \in B_m} f_i(w) + R(w)$$

Batch gradient

$$g_{B_m}(w) = \nabla_w f_{B_m}(w) = \frac{1}{m} \sum_{i \in B_m} \nabla_w f_i(w) + \nabla_w R(w)$$

B_m is a random variable $\Rightarrow f_{B_m}(w), g_{B_m}(w)$ are random variables

Unbiased Estimates: $\mathbb{E}_{B_m}\left[f_{B_m}(w)\right] = f(w), \quad \mathbb{E}_{B_m}\left[g_{B_m}(w)\right] = \nabla_w f(w)$

$g_{B_m}(w) = \nabla_w f(w) + \xi_{B_m}, \quad \mathbb{E}\left[\xi_{B_m}\right] = 0$

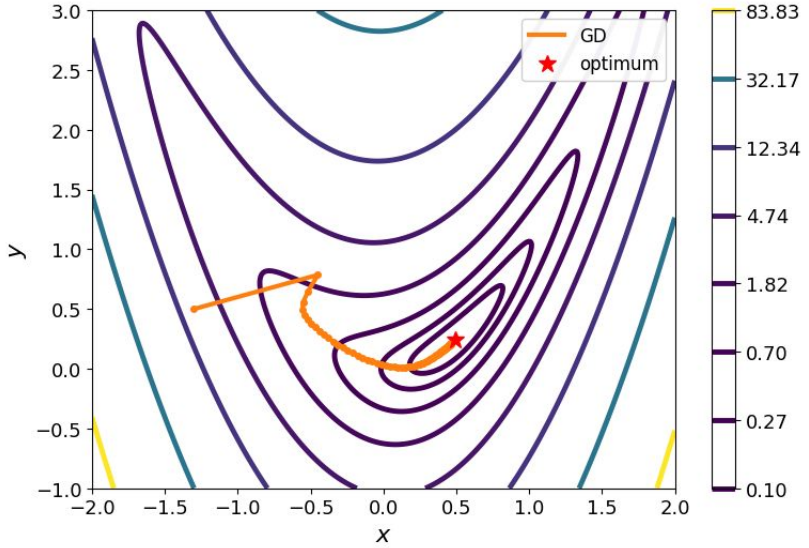
Stochastic Gradient Descent

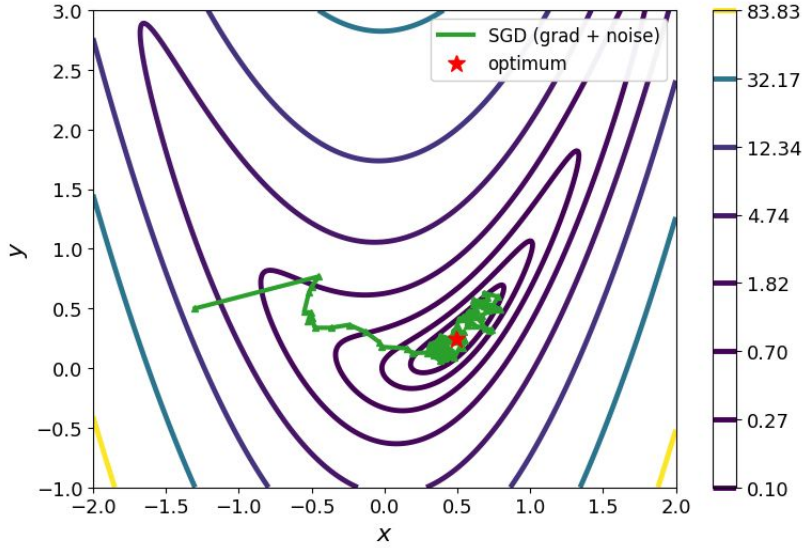
Gradient descent update

$$x_{i+1} = x_i - \alpha_i \nabla f(x_i)$$

SGD update: gradient descent with noisy gradients

$$x_{i+1} = x_i - \alpha_i g_i, \quad g_i = \nabla f(x_i) + \xi_i$$





Stochastic Gradient Descent

SGD update: gradient descent with noisy gradients

$$x_{i+1} = x_i - \alpha_i g_i, \quad g_i = \nabla f(x_i) + \xi_i$$

Assumptions:

- **strong convexity and smoothness**

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2}\|y - x\|^2,$$

$$\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\|$$

- **unbiased gradient, bounded noise variance**

$$\mathbb{E}[\xi_i \mid x_i] = 0, \quad \mathbb{E}|\xi_i|^2 \leq \sigma^2$$

- **Robbins–Monro stepsizes**

$$\alpha_i > 0, \sum_{i=1}^{\infty} \alpha_i = \infty, \quad \sum_{i=1}^{\infty} \alpha_i^2 < \infty, \quad \text{e.g. } \alpha_i = \frac{c}{i^\gamma}, \ \gamma \in (\tfrac{1}{2}, 1]$$

Sublinear convergence of iterate averages $\bar{x}_k = \frac{1}{k}\sum_{i=1}^{k} x_i$

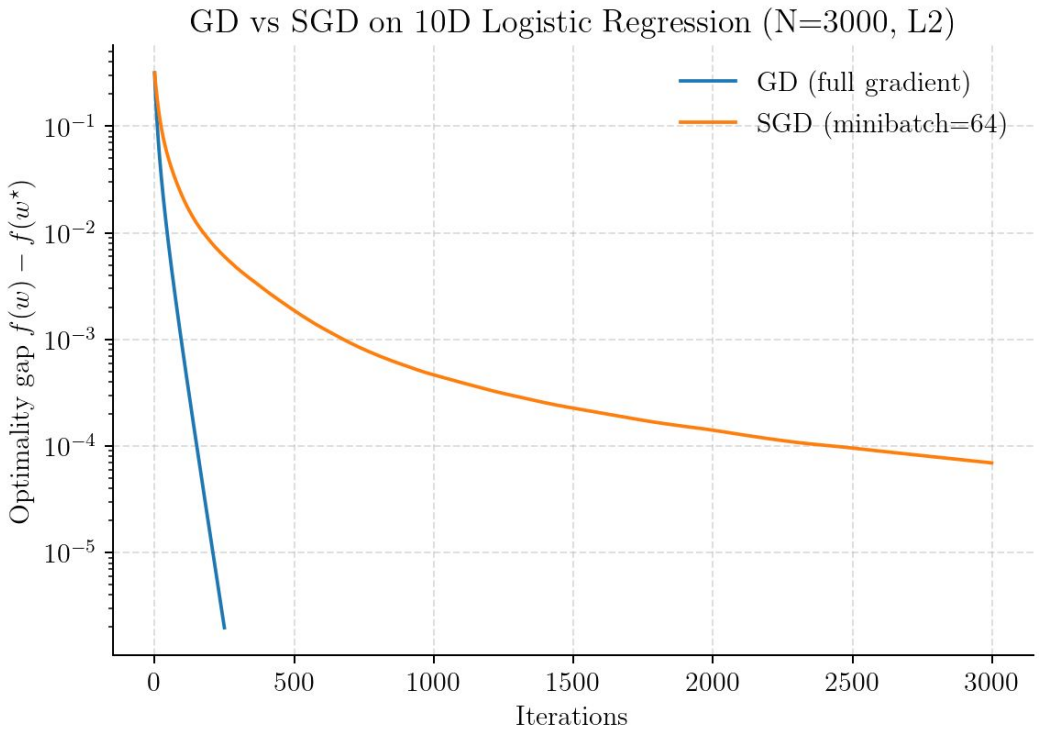
$$C = \operatorname{Tr}\left(H^{-1}\Sigma H^{-1}\right), \quad H = \nabla^2 f(x^\star), \ \Sigma = \operatorname{Cov}(\xi_i \mid x^\star)$$

$$\mathbb{E}\left\|\bar{x}_k - x^\star\right\|^2 \ \leq \ \frac{C}{k} + o\left(\tfrac{1}{k}\right),$$

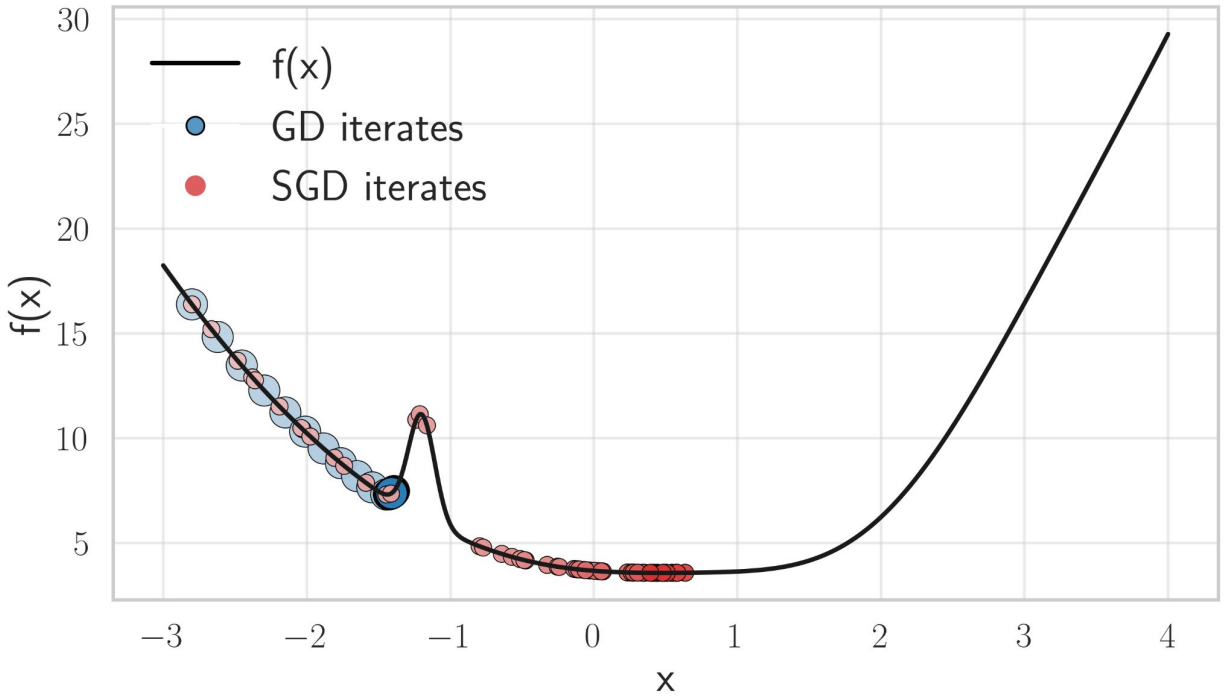
$$\mathbb{E}\left[f(\bar{x}_k) - f(x^\star)\right] \ \leq \ \tfrac{L}{2}\,\mathbb{E}\left|\bar{x}_k - x^\star\right|^2 \ = \ O\left(\tfrac{1}{k}\right)$$

$$k(\varepsilon) \text{ such that } \mathbb{E}[f(\bar{x}_k) - f(x^\star)] \leq \varepsilon \ \Leftarrow \ k(\varepsilon) = O\left(\tfrac{1}{\varepsilon}\right)$$

Stochastic Gradient Descent. Example



Is full-batch gradient descent always better?



Convex Optimization → Non-Convex Optimization

Convex functions

- Unique optimal solution (global minimum)
- Algorithms with convergence guarantess

Non-convex functions:

- Might have many optimal solutions (global minima)
- Might have many local minima
- In general, no guarantees, optimization is NP-hard
- Is there hope?
- Should we abandon ML models with non-convex loss?

Deep Learning & Optimization

Deep Learning millions/billions of parameters; Non-convex loss

Example: Image classification on ImageNet with ResNet-152

- 60 million parameters in the model
- 1 million training examples

Handwavy argument:

- If I have 60M variables and 1M equations
- I can expect to get infinite number of solutions
- Dimension of solution space: 59M = 60M - 1M

Deep Learning & Optimization & Generalization

Deep Learning millions/billions of parameters; Non-convex loss

- “Overparameterized” models
- Large number of local “solutions”
  - Shown both in theory (local optima)
  - Shown in practice (many distinct low train loss points)
- We know that some of the solutions are bad
- It is possible to find a solution where
  - Train set predictions are ~100% accurate
  - Test set predictions are completely off

Yet, Deep Networks, trained with SGD, generalize to test data in practice.

Why?

Deep Learning & Optimization & Generalization

Deep Networks, trained with SGD, generalize to test data in practice. Why?

Well, we engineered the models, and the training procedures this way

- It took a lot of time and trial and error to get Deep Networks to work
  - network architecture / initialization / learning rate schedule / …
- We selected for techniques that are likely to lead to good solutions

Model families and learning algorithms that work well have good “**inductive biases**”

- Perhaps there are “more” good solutions than bad solutions?
- Perhaps bad solutions are hard to reach with gradient descent?
  - Sharp optima / wide optima hypothesis
- Effects of overparameterization are not fully understood

Understanding optimization & generalization?

Approaches to analysing optimization & generalization in deep learning

Theoretical:

- Find set of assumption, which lead to phenomena observed in practice.
- Prove theorems about optimization & generalization under assumptions

Empirical:

- Observe interesting phenomena in practice.
- Ask questions.
- Design and run experiments.

Visualization

What is a simple thing we can do to understand optimization?

Let's visualize loss landscapes of deep networks!

1D visualization:

- Pick a 1D line in D-dimensional space
- Build a grid on the line
- Compute loss in each point on the grid

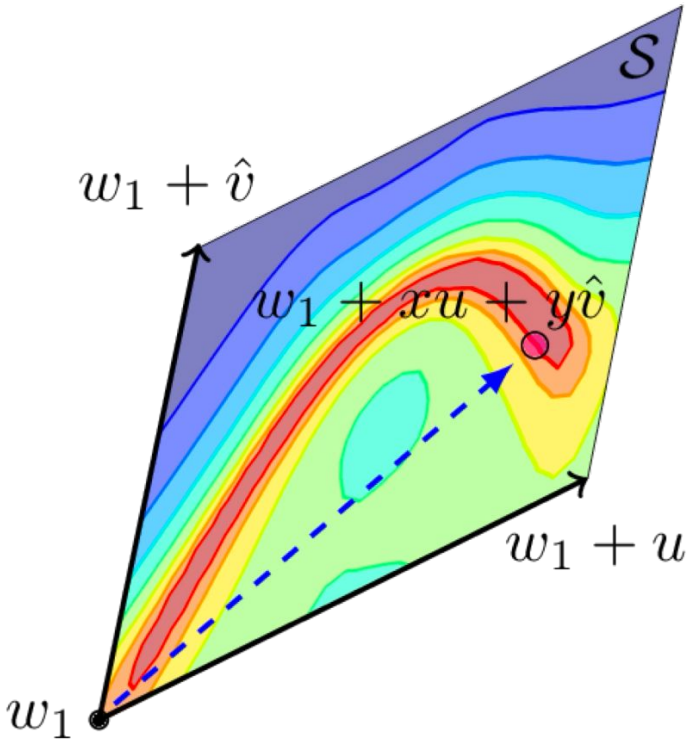
2D visualization:

- Pick a 2D plane in D-dimensional space
- Build a grid on the plane
- Compute loss in each point on the grid

We can't visualize more than 2 dimensions :-(

But we can be creative in our choice of lines/planes :-)

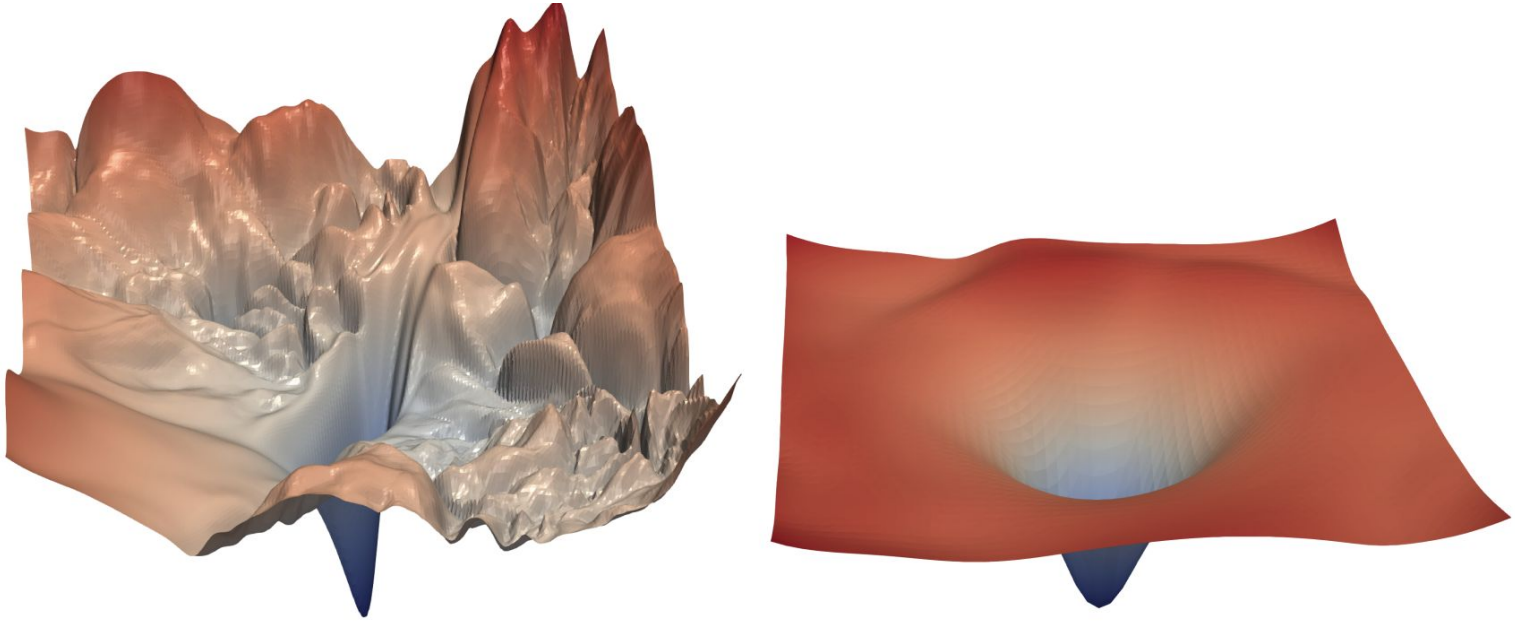
LOSS SURFACE VISUALIZATIONS



- Pick basis vectors $u, v \in \mathbb{R}^{|\text{net}|}$
- Pick a shift direction $w_1 \in \mathbb{R}^{|\text{net}|}$
- Orthogonalize: $\hat{v} = v - \dfrac{\langle v, u \rangle}{\|u\| \|v\|} u$
- Map $(x, y) \to w_1 + xu + y\hat{v}$
- Define grid in (x, y) and make a contour plot

We plot loss restricted to a 2D subspace of parameter space

Loss landscape visualizations



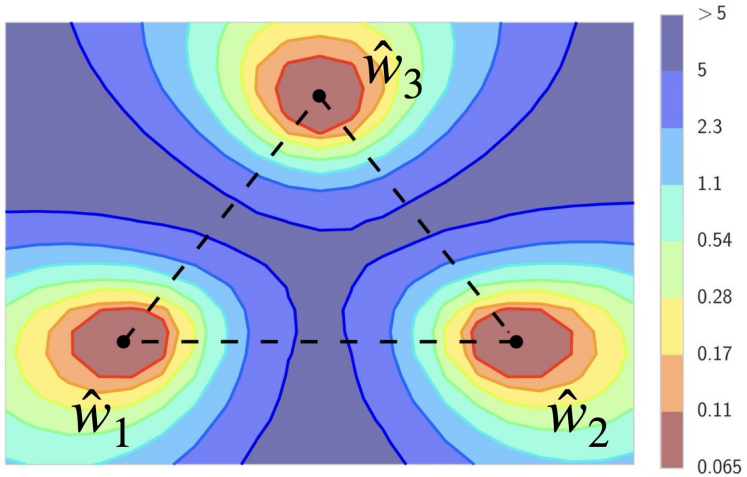
(a) without skip connections

(b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

Li et al. “Visualizing the Loss Landscape of Neural Nets”, NIPS 2018

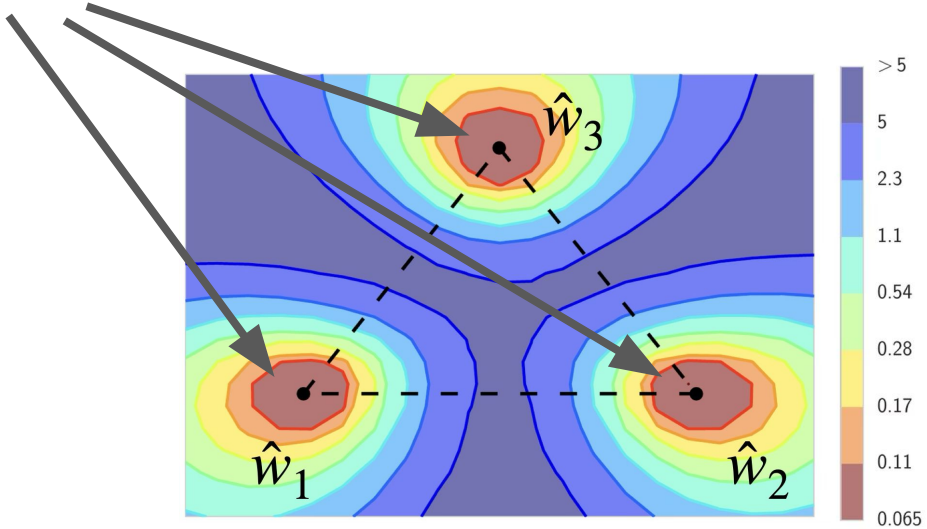
Multiple local optima



ResNet-164, CIFAR-100; train loss; 10^6 parameters

Multiple local optima

Optima ↔ similarly good, but different classifiers



Can be combined
for improved predictions
and uncertainty

ResNet-164, CIFAR-100; train loss; 10^6 parameters

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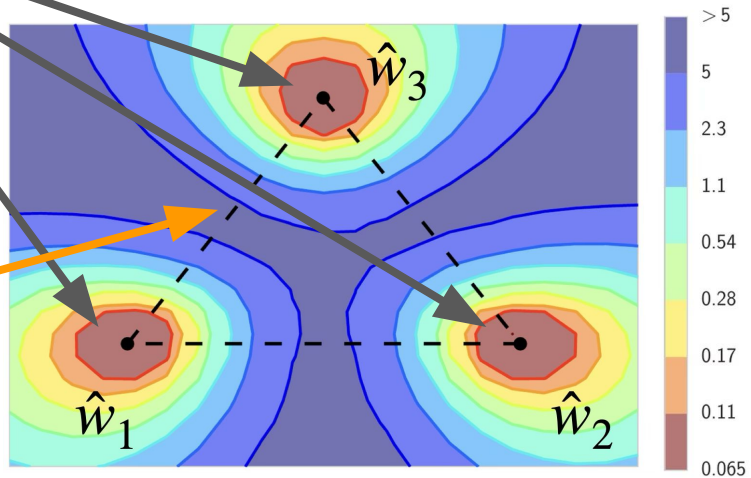


Poor loss between optima

Are optima isolated? 🤔

Can be combined
for improved predictions
and uncertainty

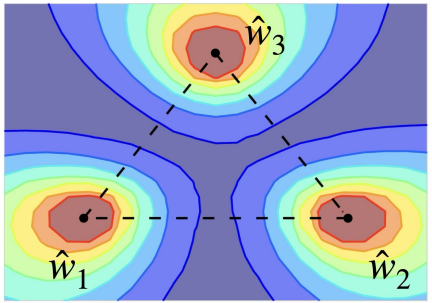
ResNet-164, CIFAR-100; train loss; 10^6 parameters

Do we need to train from scratch for diverse solutions?

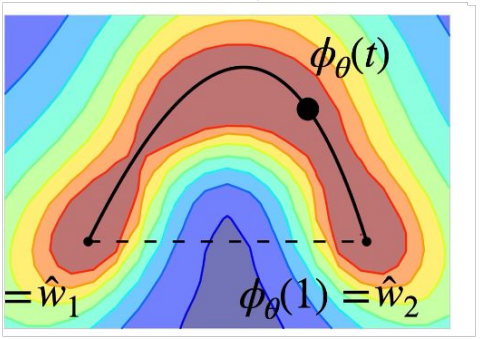
Mode connectivity

Optima are connected by simple paths of low loss!

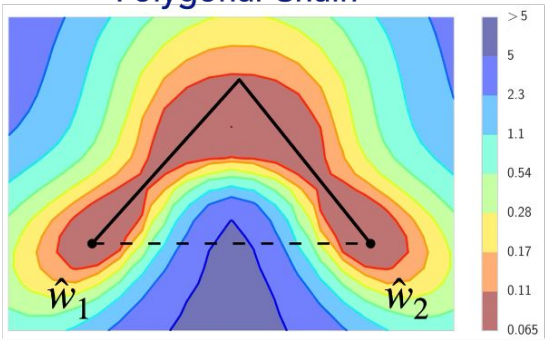
Independent Modes



Bezier Curve



Polygonal Chain

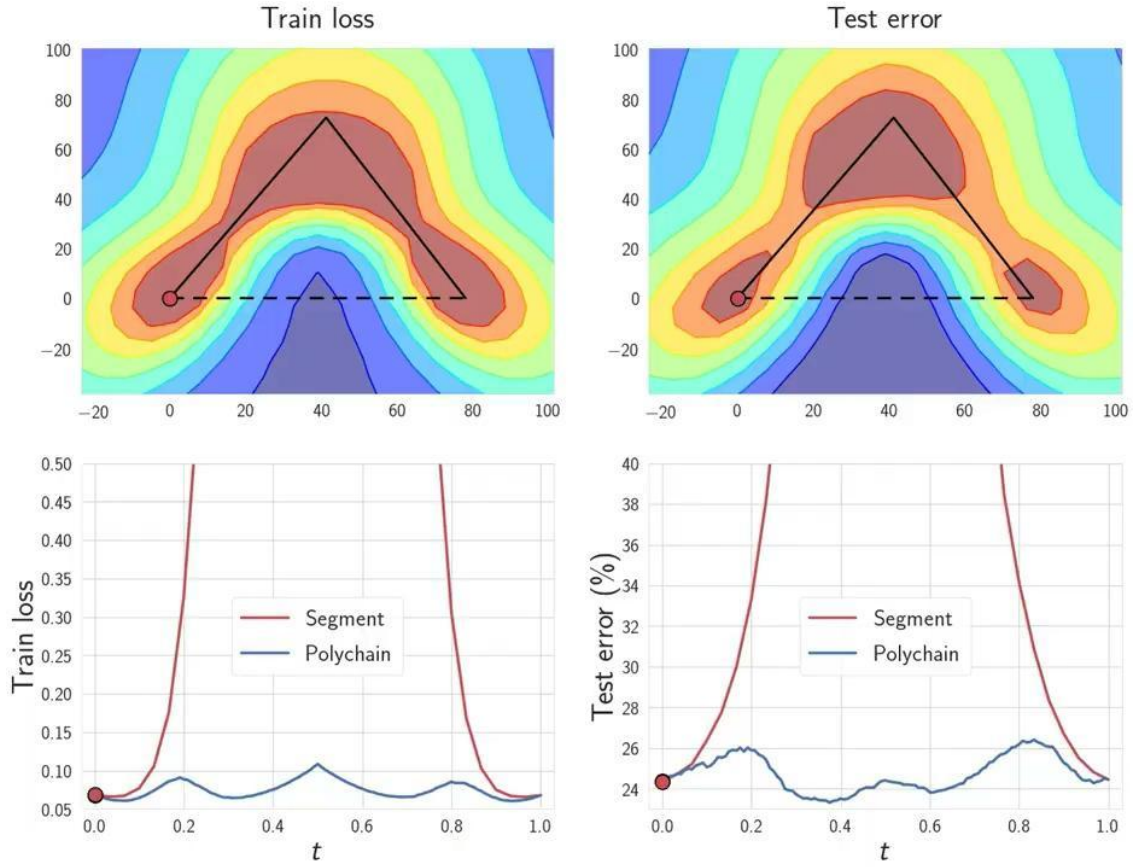


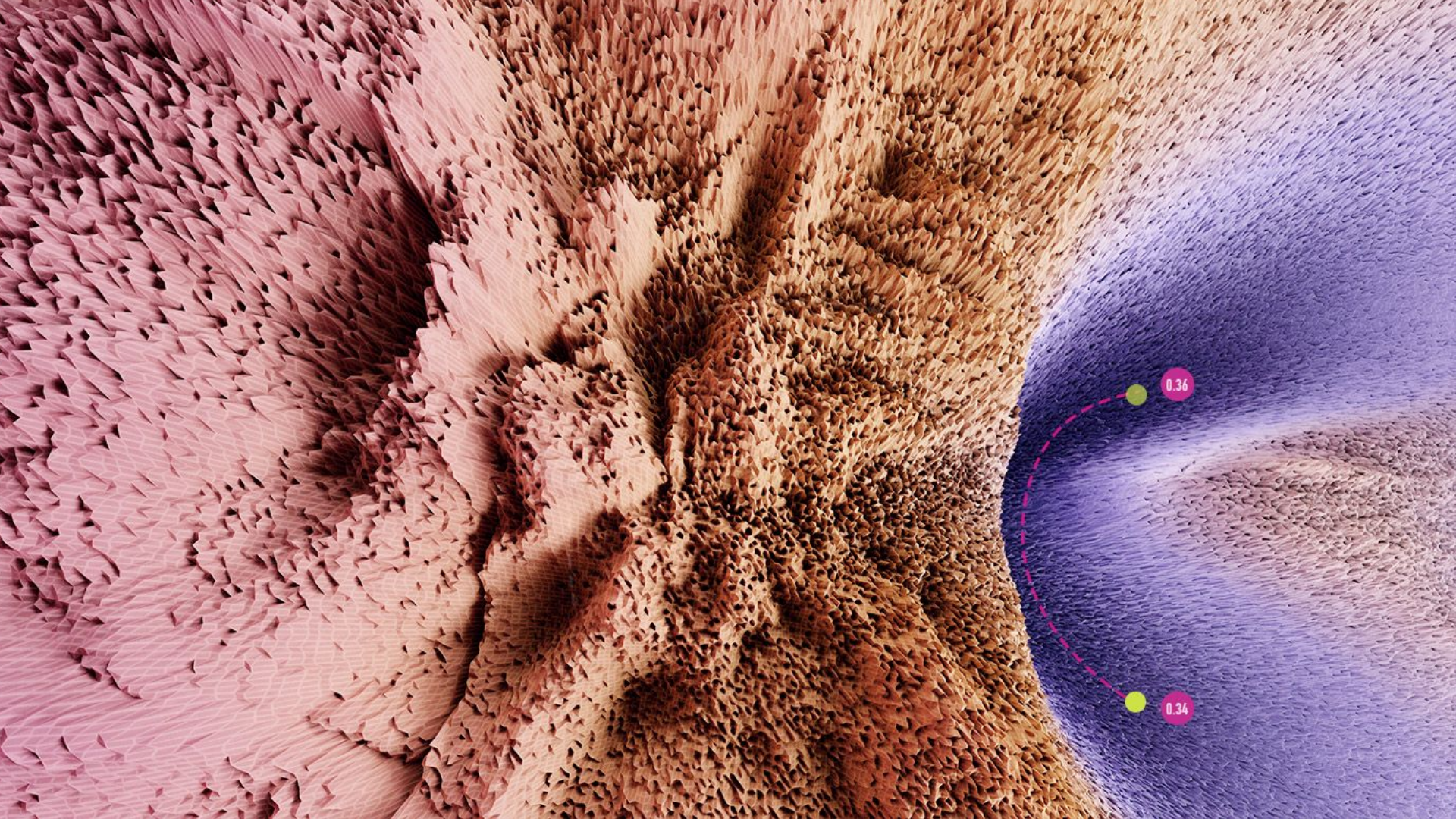
ResNet-164, CIFAR-100; train loss; 10^6 parameters

$$\phi_\theta(t) = (1-t)^2 \cdot \hat{w}_1 + 2t(1-t) \cdot \theta + t^2 \cdot \hat{w}_2$$

Minimize $\ell(\theta) = \mathbb{E}_{t\sim U[0,1]}\, L(\phi_\theta(t))$; $\quad \nabla_\theta \ell(\theta) = \mathbb{E}_{t\sim U[0,1]}\, \nabla_\theta L(\phi_\theta(t))$

Mode connectivity




0.36
0.34


Visualizations produced in collaboration with Javier Ideami
More visualizations at losslandscape.com

Flatness & Generalization

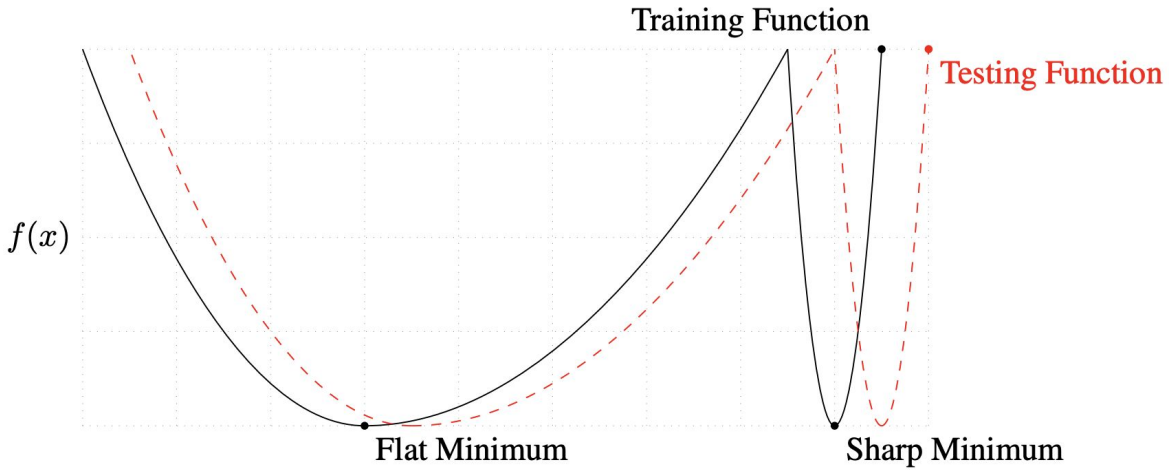
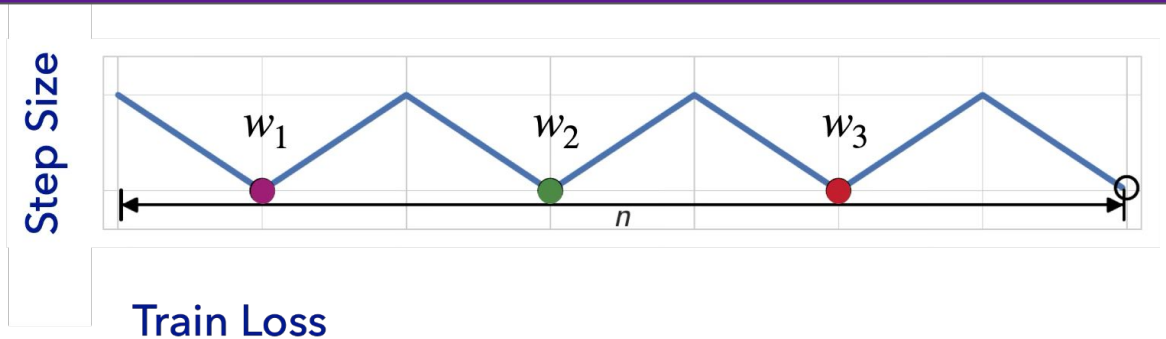


Figure 1: A Conceptual Sketch of Flat and Sharp Minima. The Y-axis indicates value of the loss function and the X-axis the variables (parameters)

Keskar et al. “On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima”, ICLR 2017

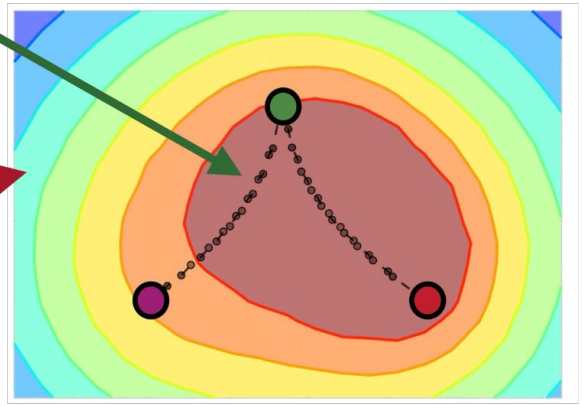
Exploring SGD trajectories



Train Loss

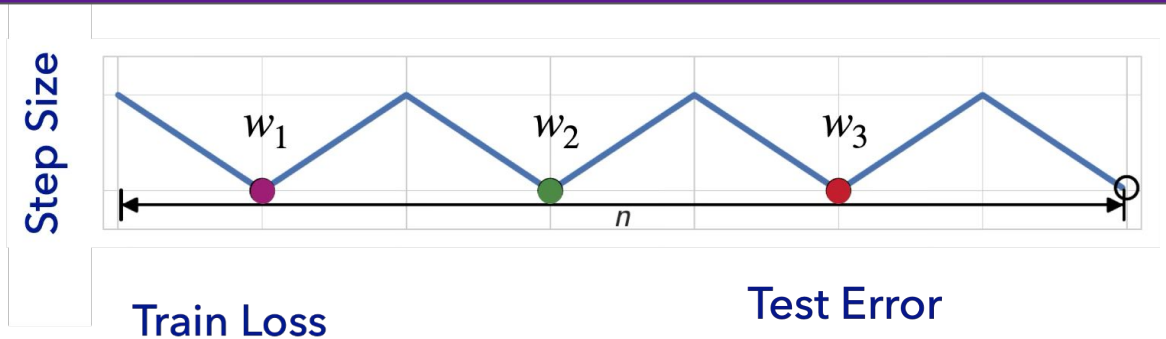
Good Region

Bad Region



ResNet-164, CIFAR-100

Exploring SGD trajectories

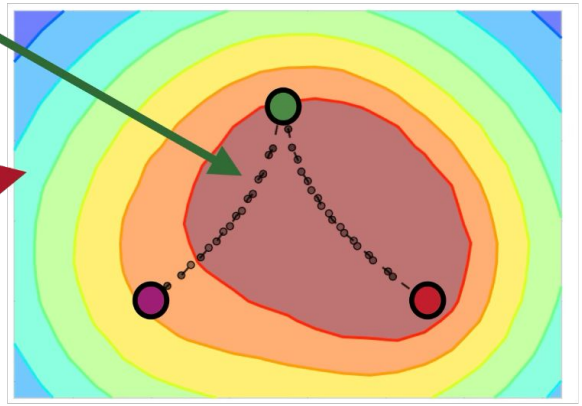


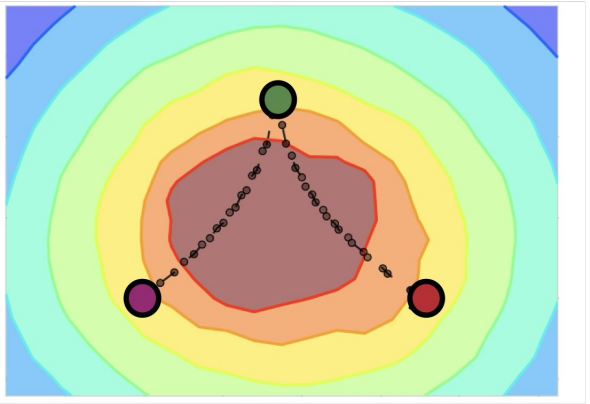
Train Loss

Test Error

Good Region

Bad Region

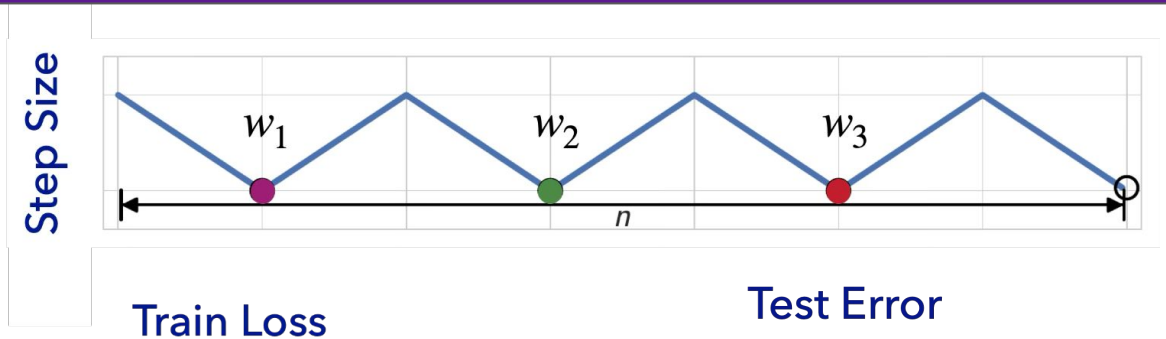




ResNet-164, CIFAR-100

Q: How to get a better model?

Exploring SGD trajectories

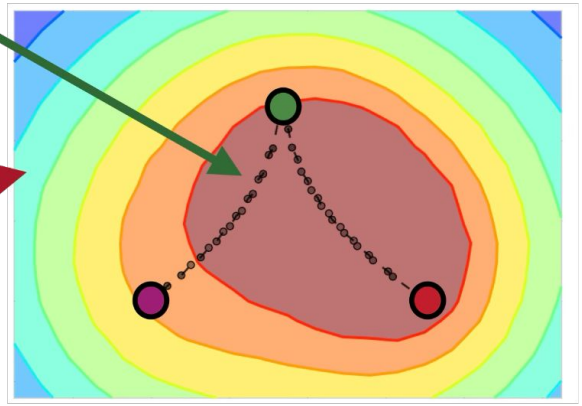


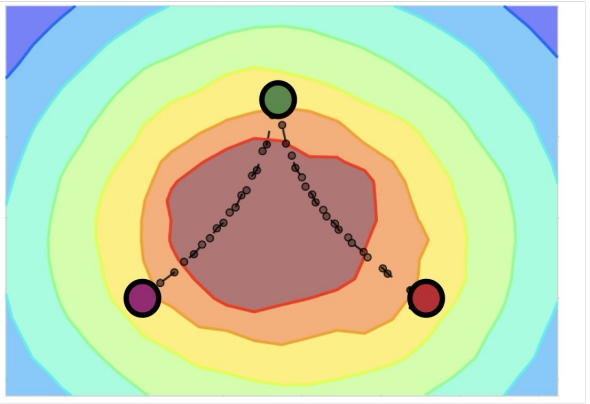
Train Loss

Test Error

Good Region

Bad Region

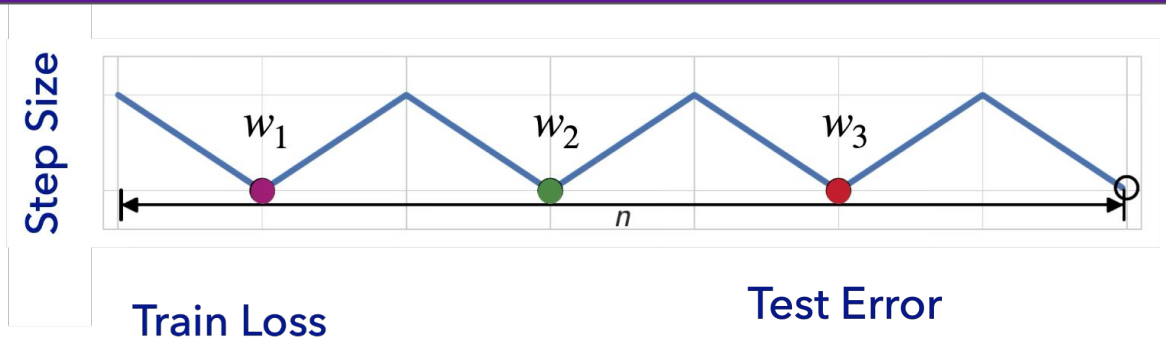




ResNet-164, CIFAR-100

Q: How to get a better model?

Exploring SGD trajectories

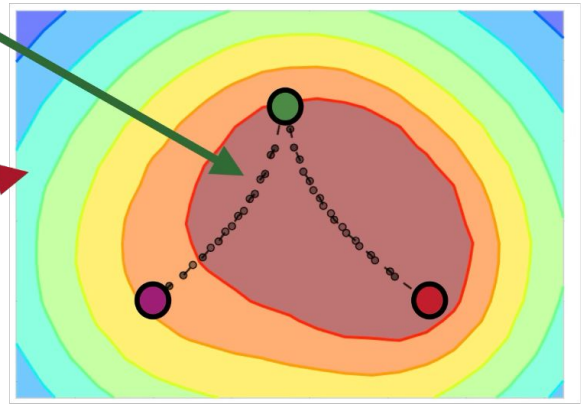


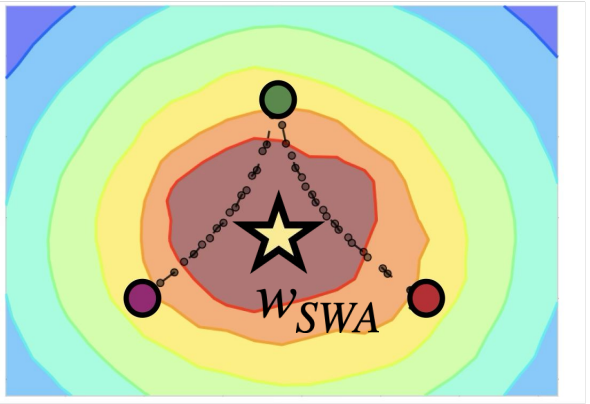
Train Loss

Test Error

Good Region

Bad Region

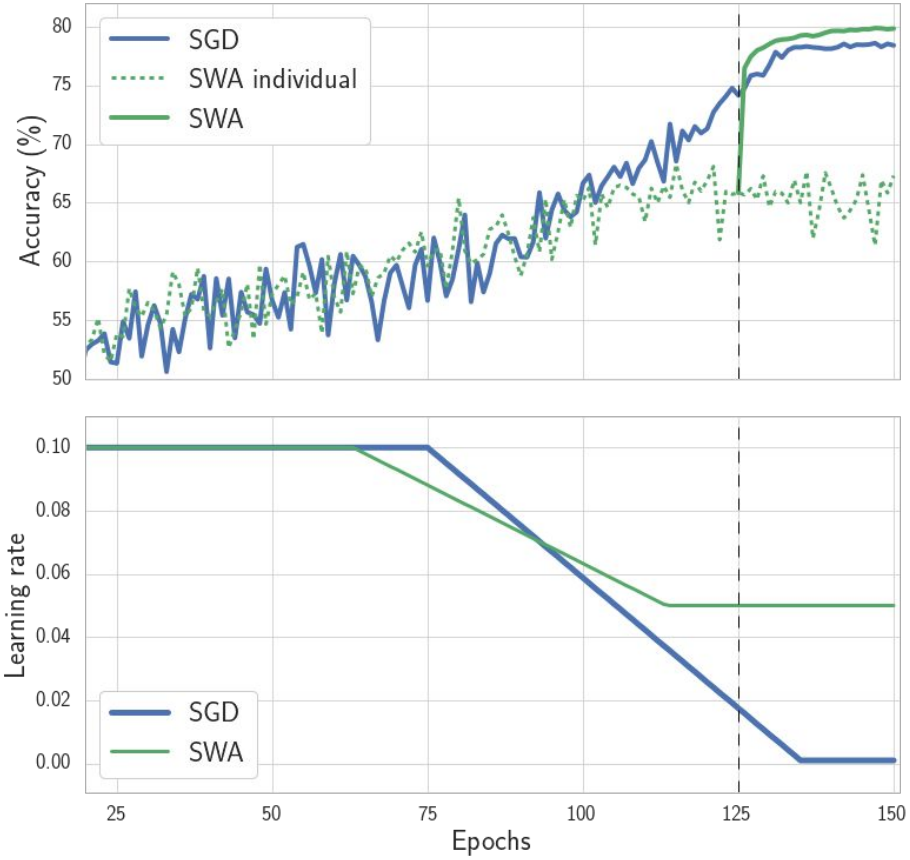




ResNet-164, CIFAR-100

Q: How to get a better model?
A: Average the weights!

Stochastic Weight Averaging (SWA) [Izmailov et al. 2018]



Model	SGD	SWA	
VGG-16	72.5 ± 0.10	**74.3 ± 0.3**	CIFAR-100
ResNet-164	78.5 ± 0.4	**80.4 ± 0.2**	
WRN-28-10	80.8 ± 0.2	**82.2 ± 0.3**	
ResNet-50	76.15	**77.0 ± 0.05**	ImageNet
DenseNet-161	77.65	**78.5 ± 0.1**	

Learning rate is important

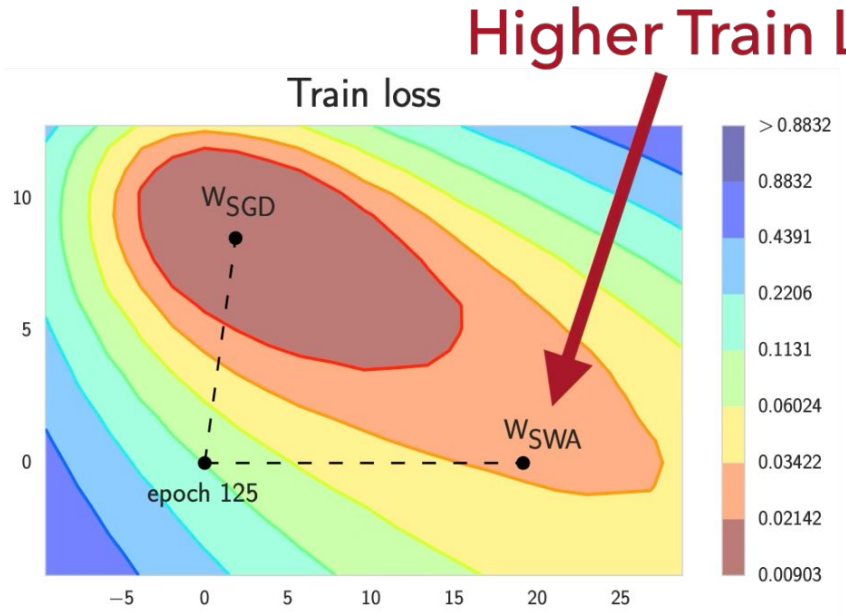
Too low learning rate:

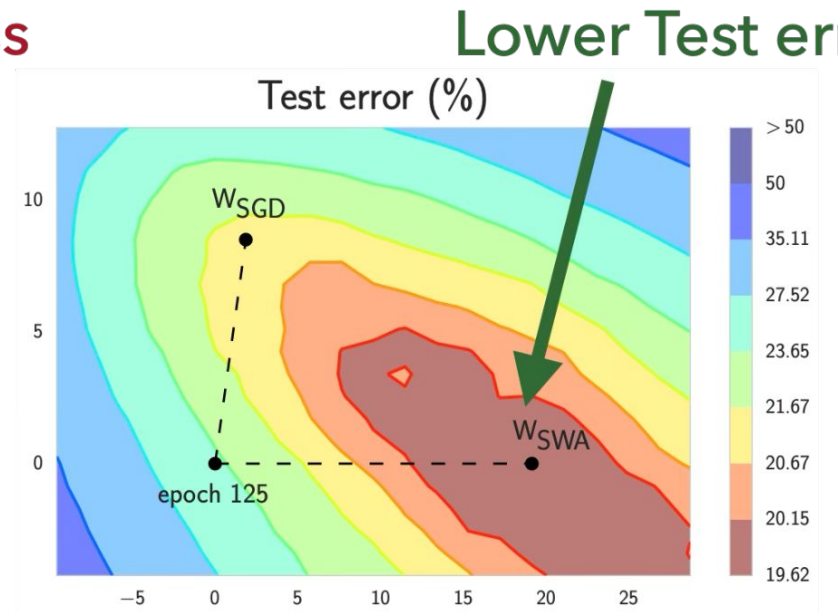
- little exploration

Too high learning rate:

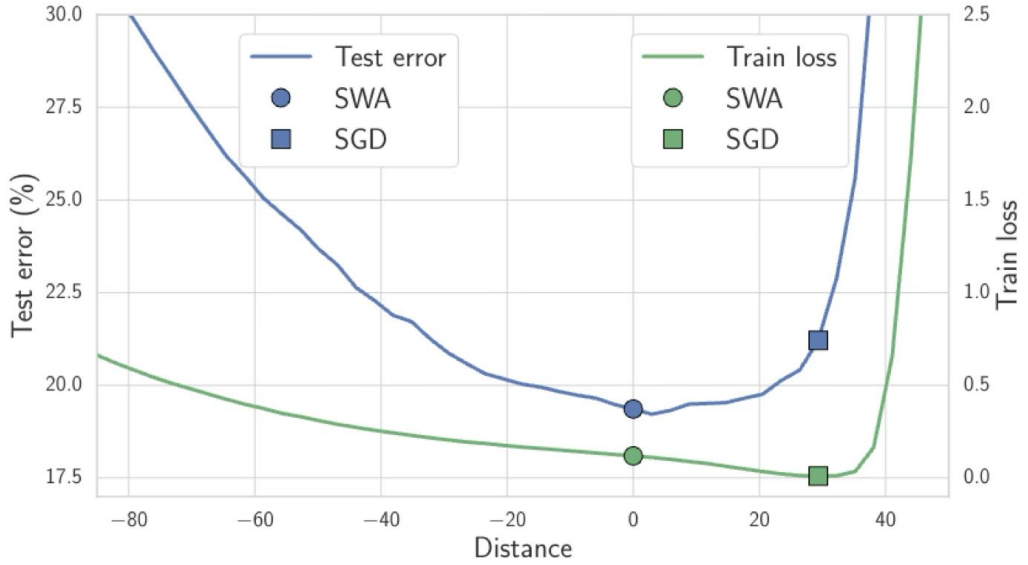
- poor individual model accuracy

Stochastic Weight Averaging (SWA) [Izmailov et al. 2018]





Stochastic Weight Averaging (SWA) [Izmailov et al. 2018]



- Train loss landscape is a **perturbed version** of test loss landscape
- SGD **overoptimizes train loss** and finds solution that is **not robust** to weight perturbations **("sharp optima")**
- Cyclical learning rate SGD **explores a local region of good solutions**
- SWA finds a **robust solution ("wide optima")**

August 18, 2020

PyTorch 1.6 now includes Stochastic Weight Averaging

```
from torch.optim import swa_utils
```

TensorFlow

TensorFlow > Resources > Addons > API

tfa.optimizers.SWA

composer

Stochastic Weight Averaging

[How to Use] - [Suggested Hyperparameters] - [Attribution] - [API Reference]

Computer Vision, Natural Language Processing

Computer Methods and Programs in Biomedicine

Volume 178, September 2019, Pages 289-301

Efficient skin lesion segmentation using separable-Unet with stochastic weight averaging

Tang Peng [a b c], Liang Qiaokang [a b c], Yan Xintong [a], Xiang Shao [a b c], Sun Wei [a b c], Zhang Dan [d], Gianmarc Coppola [e]

Benefits of Stochastic Weight Averaging in Developing Neural Network Radiation Scheme for Numerical Weather Prediction

Hwan-Jin Song, Soonyoung Roh, Juho Lee, Giung Nam, Eunggu Yun, Jongmin Yoon, Park Sa Kim

Improving Generalization of Pre-trained Language Models via Stochastic Weight Averaging

Peng Lu[1,3], Ivan Kobyzev[1], Mehdi Rezagholizadeh[1], Ahmad Rashid[1,2], Ali Ghodsi[2], Philippe Langlais[3]

Model Soups
ImageNet SOTA (2022)

Git Re-Basin
Model Fusion

SWAD | SWAP | SWAG | SWALP | TSWA

Branch-Train-Merge: Embarrassingly Parallel Training of Expert Language Models

Margaret Li*†◇ Suchin Gururangan*†◇ Tim Dettmers†

Mike Lewis◇ Tim Althoff† Noah A. Smith†♠ Luke Zettlemoyer†◇

†Paul G. Allen School of Computer Science & Engineering, University of Washington
♠Allen Institute for AI
◇Meta AI

Early Weight Averaging meets High Learning Rates for LLM Pre-training

Sunny Sanyal* UT Austin

Atula Neerkaje* UT Austin

Jean Kaddour UCL

Abhishek Kumar Google DeepMind

Sujay Sanghavi UT Austin

Google DeepMind

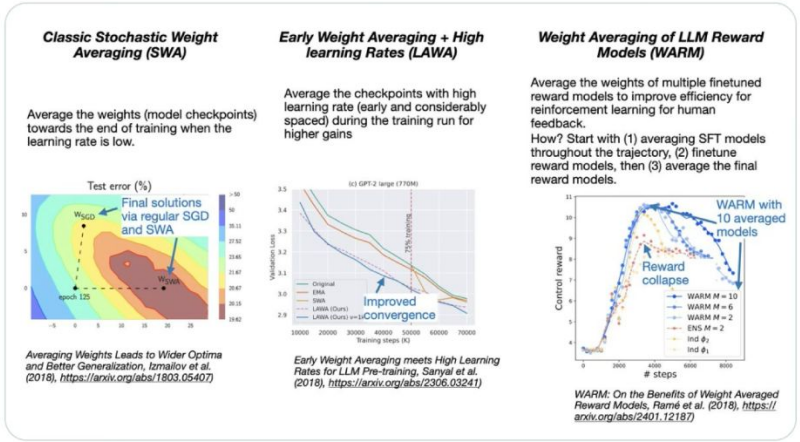
WARM: On the Benefits of Weight Averaged Reward Models

Alexandre Ramé, Nino Vieillard, Léonard Hussenot, Robert Dadashi, Geoffrey Cideron, Olivier Bachem, Johan Ferret
Google DeepMind

Sebastian Raschka ✓
@rasbt

Weight averaging and model merging for LLMs seem to be the most interesting themes in 2024 so far. What are the benefits? Combining multiple models (or checkpoints) into a single one can improve training convergence, overall performance, and also robustness.

I will probably do a deeper dive in the upcoming weeks, but here are at least 3 interesting papers. To get started, here's a selection of papers on this learning trajectory (no pun intended).



10:34 AM · Jan 24, 2024 · **151.8K** Views

21 178 1K 796

Deep Learning Loss Landscapes

“Global structure”:

- Multiple distinct local optima
- Optima are connected by non-linear paths of low loss

“Local structure”:

- SGD with non-zero LR doesn’t seem to exit linearly-connected region
- Medium-LR SGD bounces around in a wide region of low loss points
- Averaging SGD iterates helps to land in the interior of good region
- Empirically averaging finds a model that generalizes better

Still active area of research

Gradient Descent: Variations

Gradient Descent Update

$$x_{k+1} = x_k - \alpha \nabla_x f(x_k)$$

Change notation

$$\frac{x(t+dt) - x(t)}{dt} = -\nabla_x f(x(t))$$

Looks like discrete-time numerical integration of continuous time ODE

$$\dot{x}(t) = -\nabla_x f(x(t)) \qquad \text{(a.k.a. gradient flow)}$$

Physical interpretation

$x(t)$ is a trajectory of an object which moves with velocity $\dot{x}(t)$

given by the the anti-gradient vector field $v(x) = -\nabla_x f(x)$

What would change if gradient influenced acceleration instead of velocity?

Gradient Descent with Momentum

Gradient Descent Update

$$x_{k+1} = x_k - \alpha \nabla_x f(x_k)$$

What would change if gradient influenced acceleration instead of velocity?

Object with a unit mass $(m = 1)$ moves under $a = \frac{F}{m}$ in a force field $F(x) = -\nabla_x f(x)$.

$\ddot{x}(t) = -\nabla_x f(x(t))$

state of the object is described by position $x(t)$ and velocity $v(t)$.

(dynamical system with 2D state)

$$\frac{d}{dt}\begin{bmatrix} v(t) \\ x(t) \end{bmatrix} = \begin{bmatrix} -\nabla_x f(x(t)) \\ v(t) \end{bmatrix}$$

Gradient Descent with Momentum

$v_{k+1} = \beta\, v_k - \nabla_x f(x_k)$ $\quad (\beta \in [0, 1]$ — dampening)

$x_{k+1} = x_k + \alpha_k v_{k+1}$

Gradient Descent with Momentum

Gradient Descent Update

$$x_{k+1} = x_k - \alpha \nabla_x f(x_k)$$

Gradient Descent with Momentum

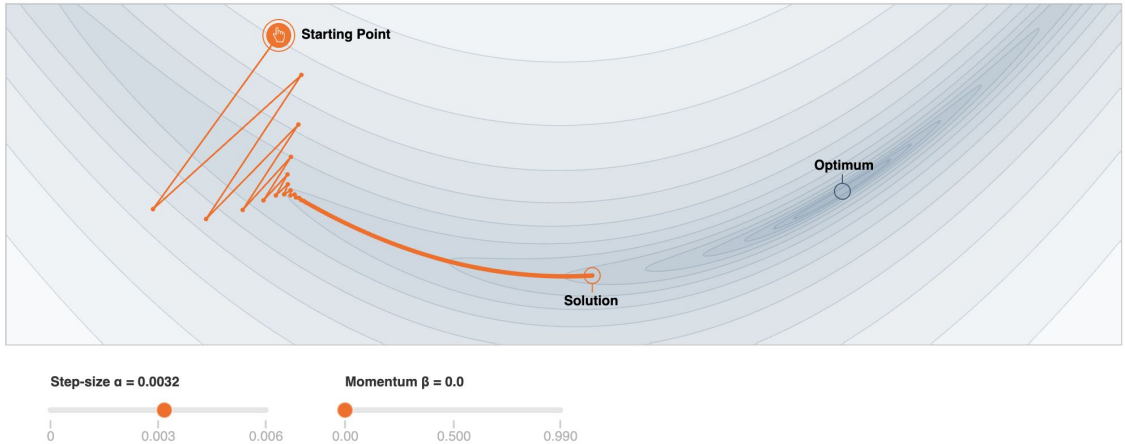
$$v_{k+1} = \beta v_k - \nabla_x f(x_k) \qquad (\beta \in [0, 1] \text{ — dampening})$$

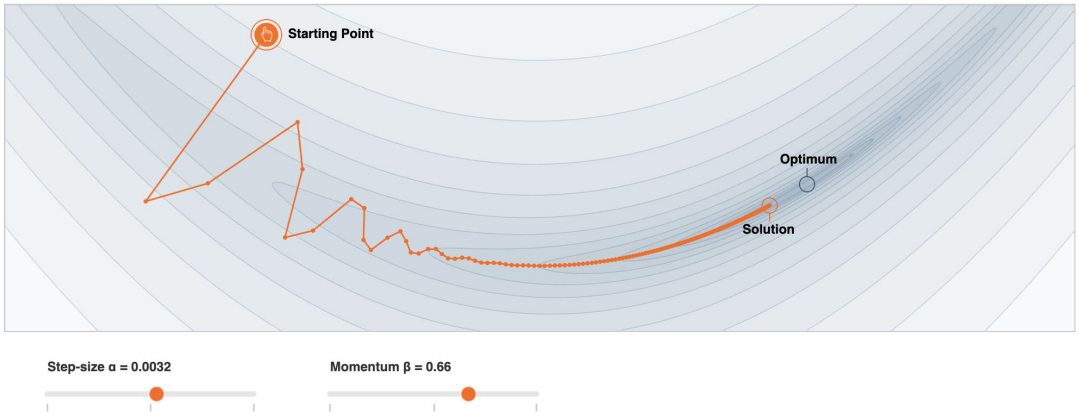
$$x_{k+1} = x_k + \alpha_k v_{k+1}$$

For strongly-convex and L-smooth functions

Linear convergence rate, but **better constant**

Visualizations by Gabriel Goh, "Why Momentum Really Works", Distill, 2017.
https://distill.pub/2017/momentum/





ADAM

ADAM [Kingma et al. 2015]

- Go-To Optimization Method for Deep Learning
- Typically optimizes loss faster than SGD
- Two ideas
  - Stochastic Gradient Descent with Momentum
  - + adaptive learning rate scale for each parameter
- Typically requires minimal hyperparameter tuning
  - Handy when experimenting with new models

Kingma et al. “Adam: A Method for Stochastic Optimization”, ICLR 2015

ADAM

for $t = 1$ **to** $\ldots$ **do**

$$g_t \leftarrow -\nabla_\theta f_t(\theta_{t-1})$$
$$m_t \leftarrow \beta_1 m_{t-1} + (1-\beta_1) g_t$$
$$v_t \leftarrow \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$
$$\widehat{m_t} \leftarrow m_t / \left(1-\beta_1^t\right)$$
$$\widehat{v_t} \leftarrow v_t / \left(1-\beta_2^t\right)$$
$$\theta_t \leftarrow \theta_{t-1} - \gamma \widehat{m_t} / \left(\sqrt{\widehat{v_t}} + \epsilon\right)$$

Notation

- t — step number
- θ_t — model parameters at step t
- g_t — gradient
- m_t — moving average of gradients (velocity)
- v_t — moving average of squared gradients

  interpretation: average (squared) gradient magnitude per parameter
- $\widehat{m_t}$, $\widehat{v_t}$ — "bias corrected" m_t and v_t
- β_1, β_2 — exponential decay rates for moving averages
- γ — learning rate
- ε — small number to prevent division by zero

Update rule

$$\theta_t = \theta_{t-1} - \gamma \frac{\widehat{m_t}}{\sqrt{\widehat{v_t} + \varepsilon}} \quad \text{(element-wise vector division)}$$

Kingma et al. "Adam: A Method for Stochastic Optimization", ICLR 2015

ADAM

Update rule

$$\theta_t = \theta_{t-1} - \gamma \frac{\widehat{m_t}}{\sqrt{\widehat{v_t} + \varepsilon}}$$

(element-wise vector division)

Notation

- m_t — moving average of gradients (velocity)
- v_t — moving average of squared gradients
  interpretation: average (squared) gradient magnitude per parameter
- $\widehat{m_t}$, $\widehat{v_t}$ — "bias corrected" m_t and v_t
- γ — learning rate
- ε — small number to prevent division by zero

Intuition:

- SGD w/momentum + adaptive per-parameter step size scaling
- Consider update for the i-th parameter $\theta[i]$
- **Large** $v_t[i] \implies$ loss is sensitive to the value of $\theta[i]$
  use **smaller step size** for $\theta[i]$ to be safe
- **Small** $v_t[i] \implies$ loss is not too sensitive to the value of $\theta[i]$
  use **larger step size** for $\theta[i]$ to move faster

Second Order Methods

$\min_{w \in \mathbb{R}^d} f(w)$ — unconstrained optimization problem in $\mathbb{R}^d$

If f is smooth, then

$$f(x_0 + h) = f(x_0) + \langle \nabla_x f(x_0), h \rangle + O(\|h\|^2)$$

The direction of the fastest descent is $h = -\nabla_x f(x_0)$

What if we use second-order approximation?

Newton's Method

If f is smooth, then

$$f(x_0 + h) = f(x_0) + \langle \nabla_x f(x_0), h \rangle + \left\langle h, \left[\nabla_x^2 f(x_0)\right] h \right\rangle + O(\|h\|^3)$$

$\left[\nabla_x^2 f(x_0)\right]$ – Hessian; d x d matrix of second derivatives

The direction of the fastest descent is $h = -\left[\nabla_x^2 f(x_0)\right]^{-1} \nabla_x f(x_0)$

Newton's Method

If f is smooth, then

$$f(x_0 + h) = f(x_0) + \langle \nabla_x f(x_0), h \rangle + \left\langle h, \left[\nabla_x^2 f(x_0)\right] h \right\rangle + O(\|h\|^3)$$

$\left[\nabla_x^2 f(x_0)\right]$ – Hessian; d x d matrix of second derivatives

The direction of the fastest descent is $h = -\left[\nabla_x^2 f(x_0)\right]^{-1} \nabla_x f(x_0)$

Newton's Method

$\min_{w \in \mathbb{R}^d} f(w)$ — unconstrained optimization problem in $\mathbb{R}^d$

Pick x_0; set $k = 0$

Until `should_stop()` :

$$x_{k+1} = x_k - \alpha_k \cdot \left[\nabla_x^2 f(x_k)\right]^{-1} \nabla_x f(x_k)$$
$$k = k + 1$$

In convex optimization

+ Super-linear convergence rate
+ Under some conditions: quadratic convergence rate
$$k(\varepsilon) = O\left(\log\log\left(\tfrac{1}{\varepsilon}\right)\right)$$
- Each step requires O(d^3) time due to matrix inversion

Quasi-Newton Methods

- Approximate Newton's direction
- e.g. L-BFGS

Second Order Methods for Large ML Models

For models with large number of parameters

- Just computing the Hessian takes O(d^2) time and memory
- Many quasi-second-order methods use cheap approximations of the Hessian
- Diagonal approximation
  - Compute only the diagonal of the Hessian
  - Takes O(d) time and memory
  - Results in per-parameter learning rate scaling
    - as in ADAM; but ADAM uses gradient history instead of Hessian
- Compressed Hessian approximations
  - Low-rank / matrix factorizations / sparse (block-sparse) / …
- Recent methods for Deep Networks
  - Shampoo [Gupta et al., 2018]
  - SOAP [Vyas et al., 2024]

Optimization in ML: Overview

Optimization is one of the tools in ML theory and practice

Theory:

- Learning as optimization
- Design & analysis of optimization algorithms, convergence guarantees
- Theoretically optimal solution → predictive model properties
    - Assuming infinite data and infinite compute, do we learn the right distribution?

$$\min_{f(\cdot)} \mathbb{E}_{p(y|x)} \left[(f(x) - y)^2 \right] \quad \Longrightarrow \quad f^*(x) = \mathbb{E}[y \mid x]$$

$$\min_{f(\cdot)} \mathbb{E}_{p(y|x)} \left[\log(1 + \exp(-y f(x))) \right] \quad \Longrightarrow \quad f^*(x) = \text{logit}(p(y \mid x))$$

Practice:

- Guidelines for parameter tuning
- Inspiration for improved methods and empirical analysis

ML is not just optimization, we care about generalization too!

Beyond Optimization

Given: training data

Want: predictive model f(x)

Learning Algorithm:

Training Data => [Algorithm] => Model

- Our primary interest is in solving learning
- Optimization is one way to look at learning algorithms
- Are there other ways?

Beyond Optimization

Learning Algorithm:

Training Data => [Algorithm] => Model

“Most general view”: dynamical systems

An algorithm running on a computer is a dynamical system

- Memory = state
- Program = update rule

$$s_{t+1} = F(s_t)$$

Cannot get more general than that :-)

Instead of thinking about design of loss function and optimization algorithm

We can think about design of dynamical system

Optimization $\subset$ Dynamical Systems

Continuous **optimization**

Model Parameters & **Loss Function** → **Gradient** Vector Field → Update Rule

$$x_{t+1} = x_t + V(x_t), \quad V(x_t) = -\nabla_x \operatorname{Loss}(x_t)$$

- V(x) is called a “conservative” vector field in calculus / physics
- -Loss(x) is the “potential” of V(x)

Continuous **dynamical system**

Model Parameters → Vector Field → Update Rule

$$x_{t+1} = x_t + V(x_t)$$

Let’s come up with interesting non-conservative vector fields!

Optimization $\subset$ Game Theory

Optimization:

- One group of parameters
- Minimizing one loss function
- Solution: minimizer

$$\min_x U(x) \quad \Rightarrow \quad V(x) = -\nabla_x U(x) \quad \Rightarrow \quad x_t = x_t - \alpha_t \nabla_x U(x_t)$$

Game:

- Multiple groups of parameters (players)
- Each player minimizes its own loss function (other terminology: maximizing utility fn)
- Solution: equilibrium point
  - E.g. Nash equilibrium

$$\begin{aligned} &\min_{x_1} U_1(x_1, x_2) \\ &\min_{x_2} U_2(x_1, x_2) \end{aligned} \quad \Rightarrow \quad V\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} -\nabla_{x_1} U_1(x_1, x_2) \\ -\nabla_{x_2} U_2(x_1, x_2) \end{bmatrix} \quad \Rightarrow$$

Simultaneous Gradient Descent

$$\begin{aligned} x_{1,t+1} &= x_{1,t} - \alpha_t \nabla_{x_1} U_1(x_{1,t}, x_{2,t}) \\ x_{2,t+1} &= x_{2,t} - \alpha_t \nabla_{x_2} U_2(x_{1,t}, x_{2,t}) \end{aligned}$$

Games in ML. Example: GANs

Generative Adversarial Networks (GANs)

- Generative model
- Goal:
  - Given a dataset of examples (e.g. images)
  - Learn to generate new examples (e.g. new realistic images)

GAN: 2-player Game

- Generator Network:
  - Takes random noise as an input, produces an image
- Discriminator Network:
  - Takes image as an input; outputs a probability score
  - D(x) = probability of x being a real image

Goodfellow et al. “Generative Adversarial Networks”, NIPS 2014

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Loss functions:

- Discriminator loss: classification loss; classify if input x is a real or fake image
- Generator loss: opposite of discriminator loss
  - Generator gets low loss if discriminator thinks that generated image is “real”

Nash equilibrium:

- G* – Generator that perfectly learns the training data distribution
- D* – Discriminator that outputs 0.5 for any input

Goodfellow et al. “Generative Adversarial Networks”, NIPS 2014