Interpolation, Growth Conditions, and Stochastic Gradient Descent

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Training neural networks is dangerous work!





Chapter 1: Introduction

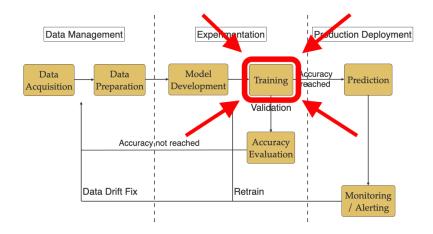
Chapter 1: Goal

Premise: modern neural networks are extremely flexible and can exactly fit many training datasets.

- e.g. ResNet on CIFAR-10, SVHN, BERT on DBpedia etc.
- Empirically, optimization is "faster than it should be".

Question: what is the complexity of learning these models using stochastic gradient descent (SGD)?

Chapter 1: Model Fitting in ML



https://towards datascience.com/challenges-deploying-machine-learning-models-to-production-ded 3 f 9009 cb3

Chapter 1: Stochastic Gradient Descent

"Stochastic gradient descent (SGD) is today one of the main workhorses for solving large-scale supervised learning and optimization problems."

—Drori and Shamir [2019]

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Chapter 1: Consensus Says. . .

... and also Agarwal et al. [2017], Assran and Rabbat [2020], Assran et al. [2018], Bernstein et al. [2018], Damaskinos et al. [2019], Geffner and Domke [2019], Gower et al. [2019], Grosse and Salakhudinov [2015], Hofmann et al. [2015], Kawaguchi and Lu [2020], Li et al. [2019], Patterson and Gibson [2017], Pillaud-Vivien et al. [2018], Xu et al. [2017], Zhang et al. [2016]

Chapter 1: Challenges in Optimization for ML

Stochastic gradient methods are the most popular algorithms for fitting ML models,

SGD:
$$w_{k+1} = w_k - \eta_k \nabla f_i(w_k)$$
.

But practitioners face major challenges with

- **Speed**: step-size/averaging controls convergence rate.
- Stability: hyper-parameters must be tuned carefully.
- **Generalization**: optimizers encode statistical tradeoffs.

Chapter 1: Challenges in Optimization for ML

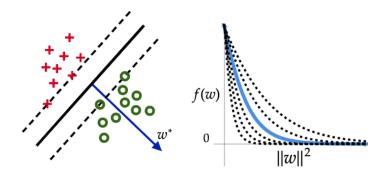
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Chapter 1: Better Optimization via Better Models



Idea: exploit "over-parameterization" for better optimization.

- Intuitively, gradient noise goes to 0 if all data are fit exactly.
- No need for decreasing step-sizes, or averaging for convergence.

Chapter 2: Interpolation and Growth Conditions

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 $\forall w \in \mathbb{R}^d$,

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- Non-negative losses like squared-error and cross-entropy.
- f is L-smooth: $w \mapsto \nabla f(w)$ is L-Lipschitz,

$$\|\nabla f(w) - \nabla f(u)\|_2 \le L\|w - u\|_2 \qquad \forall w, u \in \mathbb{R}^d,$$

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- Gradient for squared-error, cross-entropy is (sub) linear.
- (Optional) f is μ -strongly-convex: $\exists \mu \geq 0$ such that,

$$f(u) \ge f(w) + \langle \nabla f(w), u - w \rangle + \frac{\mu}{2} ||u - w||_2^2 \quad \forall w, u \in \mathbb{R}^d.$$

▶ Squared-error if $n \ge d$ and examples are linearly indep.

Stochastic Oracles:

1. At each iteration k, query oracle $\mathcal O$ for stochastic estimates

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4. \mathcal{O} is **individually-smooth**, meaning $f(\cdot, z_k)$ is L_{max} -smooth,

$$\|\nabla f(w, z_k) - \nabla f(u, z_k)\|_2 \le L_{\max} \|w - u\|_2 \quad \forall w, u \in \mathbb{R}^d,$$

almost surely.

Chapter 2: Defining Interpolation

Definition (Interpolation: Minimizers)

$$(f,\mathcal{O})$$
 satisfies minimizer interpolation if

$$w' \in \arg\min f \implies w' \in \arg\min f(\cdot, z_k)$$
 a.s.

Definition (Interpolation: Stationary Points)

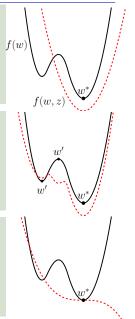
$$(f,\mathcal{O})$$
 satisfies stationary-point interpolation if

$$\nabla f(w') = 0 \implies \nabla f(w', z_k) \stackrel{\text{a.s.}}{=} 0.$$

Definition (Interpolation: Mixed)

$$(f,\mathcal{O})$$
 satisfies mixed interpolation if

$$w' \in \arg\min f \implies \nabla f(w', z_k) \stackrel{\text{a.s.}}{=} 0.$$



Chapter 2: Interpolation Relationships

- Not trivial in higher dimensions.
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- We formally define them and characterize their relationships.

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Lemma (Interpolation Relationships)

Let (f, \mathcal{O}) be arbitrary. Then only the following relationships hold:

 ${\it Minimizer\ Interpolation} \implies {\it Mixed\ Interpolation}$ and

Stationary-Point Interpolation \implies Mixed Interpolation.

However, if f and $f(\cdot, z_k)$ are invex (almost surely) for all k, then the three definitions are equivalent.

Note: invexity is weaker than convexity and implied by it.

Chapter 2: Using Interpolation

There are two obvious ways that we can leverage interpolation:

- 1. Relate interpolation to **global behavior** of \mathcal{O} .
 - ► This was first done using the weak and strong growth conditions by Vaswani et al. [2019a].
- 2. Use interpolation in a direct analysis of SGD.
 - ► This was first done by Bassily et al. [2018], who analyzed SGD under a curvature condition.

We do both, starting with weak/strong growth.

Growth Conditions: Well-behaved Oracles

There are many possible regularity assumptions on \mathcal{O} .

Bounded Gradients :
$$\mathbb{E}\left[\|\nabla f(w, z_k)\|^2\right] \leq \sigma^2$$
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Bounded Variance:
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Strong Growth+Noise :
$$\mathbb{E}\left[\|\nabla f(w, z_k)\|^2\right] \leq \rho \|\nabla f(w)\|^2 + \sigma^2$$
.

ullet Satisfied when ${\mathcal O}$ is individually-smooth and bounded below.

Growth Conditions: Strong and Weak Growth

We obtain the strong and weak growth conditions as follows:

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Strong Growth :
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Weak Growth:
$$\mathbb{E}\left[\|\nabla f(w, z_k)\|^2\right] \le \alpha \left(f(w) - f(w^*)\right)$$
.

• Implies **mixed** interpolation.

Growth Conditions: Interpolation + Smoothness

Lemma (Interpolation and Weak Growth)

Assume f is L-smooth and $\mathcal O$ is L_{\max} individually-smooth. If minimizer interpolation holds, then weak growth also holds with $\alpha \leq \frac{L_{\max}}{L}$.



Lemma (Interpolation and Strong Growth)

Assume f is L-smooth and μ strongly-convex and $\mathcal O$ is L_{\max} individually-smooth. If minimizer interpolation holds, then strong growth also holds with $\rho \leq \frac{L_{\max}}{u}$.

Comments:

- This improves on the original result by Vaswani et al. [2019a], which required convexity.
- Oracle framework extends relationship beyond finite-sums.
- See thesis for additional results on weak/strong growth.

Chapter 3: Stochastic Gradient Descent

Chapter 3: Fixed Step-size SGD

Fixed Step-Size SGD

- 0. Choose an initial point $w_0 \in \mathbb{R}^d$.
- 1. For each iteration k > 0:
 - 1.1 Query \mathcal{O} for $\nabla f(w_k, z_k)$.
 - 1.2 Update input as

$$w_{k+1} = w_k - \eta \nabla f(w_k, z_k).$$

Chapter 3: Fixed Step-size SGD

Prior work for SGD under growth conditions or interpolation:

- Convergence under strong growth [Cevher and Vu, 2019, Schmidt and Le Roux, 2013, Solodov, 1998, Tseng, 1998].
- Convergence under weak growth [Vaswani et al., 2019a].
- Convergence under interpolation [Bassily et al., 2018].

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- Convergence under interpolation [Bassily et al., 2018].

We provide many new and improved results:

- Bigger step-sizes and faster rates for convex and strongly-convex objectives.
- Almost-sure convergence under weak/strong growth.
- Trade-offs between growth conditions and interpolation.

Chapter 4: Line Search

Chapter 4: Weakness of Fixed Step-size SGD

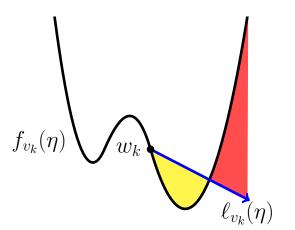
Problem: these convergence rates for fixed step-size SGD rely on using the optimal step-size, which depends on $L_{\rm max}$, α , or ρ .

Is **grid-search** really the best way to pick η ?

SGD: the Armijo Line-search

The **Armijo line-search** is a classic solution to step-size selection.

$$f(\underbrace{w_k - \eta_k \nabla f(w_k)}_{w_{k+1}}) \le f(w_k) - c \cdot \eta_k \|\nabla f(w_k)\|^2.$$



SGD with Armijo Line-search: Procedure

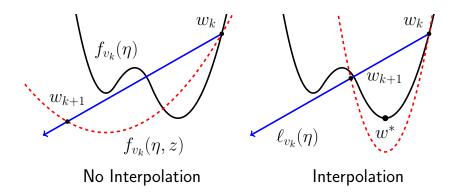
SGD with Armijo Line-Search

- 0. Choose an initial point $w_0 \in \mathbb{R}^d$.
- 1. For each iteration *k*:
 - 1.1 Query \mathcal{O} for $f(w_k, z_k)$, $\nabla f(w_k, z_k)$.
 - 1.2 Set $w_{k+1} \leftarrow w_k \eta_k \nabla f(w_k, z_k)$.
 - 1.3 Backtrack (decrease η_k) until

$$f(w_{k+1}, z_k) \le f(w_k, z_k) - c \cdot \eta_k \|\nabla f(w_k, z_k)\|^2.$$

Note: Evaluates Armijo condition on $f(\cdot, z_k)$ instead of f and needs direct access to $f(\cdot, z_k)$ to backtrack.

SGD with Armijo Line-search: Visualization



SGD with Armijo Line-search: Key Lemma

Lemma (Step-size Bound)

Assume f is L-smooth and \mathcal{O} is L_{\max} individually-smooth. Assume minimizer interpolation holds.

Then the **maximal** step-size satisfying the stochastic Armijo condition satisfies the following:

$$\frac{2(1-c)}{L_{\max}} \leq \eta_{\max} \leq \frac{f(w_k, z_k) - f(w^*, z_k)}{c\|\nabla f(w_k, z_k)\|^2}.$$









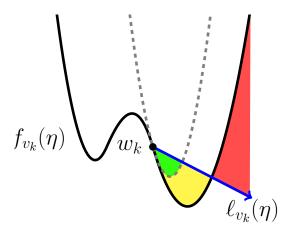


Comments:

- Mirrors classic result in deterministic optimization.
- Easy to relax to a backtracking line-search.

SGD with Armijo Line-Search: Lemma Geometry

$$\frac{2(1-c)}{L_{\max}} \le \eta_{\max} \le \frac{f(w_k, z_k) - f(w^*, z_k)}{c \|\nabla f(w_k, z_k)\|^2}.$$



SGD with Armijo Line-search: Convergence

Theorem (Convex + Interpolation)

Assume f is convex, L-smooth and $\mathcal O$ is L_{\max} individually-smooth. Assume minimizer interpolation holds and $f(\cdot,z_k)$ is almost-surely convex for all k. Then SGD with the Armijo line-search and $c=\frac{1}{2}$ converges as

$$\mathbb{E}\left[f(\bar{w}_K)\right] - f(w^*) \le \frac{L_{\max}}{2K} \|w_0 - w^*\|^2.$$

Comments:

- Improves constants in original result [Vaswani et al., 2019b]
 line-search is just as fast as the best constant step-size!
- Using the Armijo line-search is (nearly) parameter-free and recovers the deterministic rate when $L_{\max} = L$.
- See thesis for strongly-convex rate (improves $\bar{\mu}$ to μ).

Chapter 5: Acceleration

Chapters 5 and 6: Acceleration

SGD can be accelerated when minimizer interpolation holds:

- Liu and Belkin [2020] modify Nesterov's method and analyze convergence for strongly-convex functions.
- Vaswani et al. [2019a] analyze Nesterov's method under strong growth for strongly-convex and convex functions.

We follow Vaswani et al. [2019a], but provide tighter rates.

- Improves dependence on the strong-growth parameter from ρ to $\sqrt{\rho}$ factor of $\sqrt{L_{\rm max}/\mu}$ in the worst case.
- Analysis proceeds via estimating sequences; details in thesis.

Takeaways

- **Interpolation**: the oracle model extends interpolation to general stochastic optimization problems.
- Growth Conditions: "smooth" oracles satisfying interpolation are well-behaved globally.
- **SGD**: improved rates show SGD under interpolation is tight with the deterministic case.
- Line-Search: the Armijo line-search yields fast, parameter-free optimization under interpolation.
- Acceleration: stochastic acceleration is possible with a penalty of only $\sqrt{\rho}$.

Thanks for Listening!

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Left to right: Sharan Vaswani, Issam Laradji, Gauthier Gidel, Mark Schmidt, Simon Lacoste-Julien, Frederik Kunstner, Si Yi Meng, Jonathan Lavington, Yihan Zhou, and Betty Shea.

Bonus: SFOs and Least Squares

Least Squares :
$$w^* \in \arg\min \frac{1}{2n} \sum_{i=1}^{n} (\langle w, x_i \rangle - y_i)^2$$
.

The **sub-sampling** oracle sets $z_k \sim \mathsf{Uniform}(1,\ldots,n)$ and returns

$$f(w, z_k) = \frac{1}{2} \left(\langle w, x_i \rangle - y_i \right)^2$$
 and $\nabla f(w_k, z_k) = \left(\langle w, x_i \rangle - y_i \right) x_i$.

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Observations:

- O is unbiased.
- \mathcal{O} is $L_{\mathsf{max}} = \max_i \|x_i\|_2^2$ individually-smooth since

$$f_i(w) = \frac{1}{2} \left(\langle w, x_i \rangle - y_i \right)^2,$$

is $||x_i||_2^2$ -smooth for each $i \in [n]$.

Bonus: Convergence for Fixed Step-size SGD

Theorem (Convex + Weak Growth)

Assume f is convex, L-smooth and (f,\mathcal{O}) satisfies weak growth. Then SGD with $\eta=\frac{1}{2\alpha L}$ converges as

$$\mathbb{E}[f(\bar{w}_K)] - f(w^*) \le \frac{2\alpha L}{K} ||w_0 - w^*||^2.$$

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Assume f is convex, L-smooth and $\mathcal O$ is L_{\max} individually-smooth. Assume minimizer interpolation holds. Then SGD with $\eta=\frac{1}{L_{\max}}$ converges as

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Bonus: Trade-offs

Weak Growth :
$$\mathbb{E}\left[f(\bar{w}_K)\right] - f(w^*) \leq \frac{2\alpha L}{K}\|w_0 - w^*\|^2.$$
 V.S.

Interpolation :
$$\mathbb{E}\left[f(\bar{w}_K)\right] - f(w^*) \leq \frac{L_{\text{max}}}{2K} \|w_0 - w^*\|^2$$
.

Comments:

• By minimizer interpolation and individual-smoothness,

$$\alpha \leq \frac{L_{\max}}{L}.$$

- So, the second rate is better than the first in the worst-case!
- If $L_{\text{max}} = L$, then the second rate is tight deterministic GD!

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