CSC 2541: Neural Net Training Dynamics Lecture 10 - Differentiable Games

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• So far, we have been exclusively discussing minimization problems:

$$\mathbf{z}^* \in \operatorname*{arg\,min}_{\mathbf{z}} f(\mathbf{z})$$

(minimizing a single objective)

• What if we have multiple players and each of them optimizes their own objective?

$$\mathbf{z}_i^* \in \operatorname*{arg\,min}_{\mathbf{z}_i} f_i(\mathbf{z}_i, \mathbf{z}_{-i}^*)$$

(now, we're trying to find local/global Nash equilibrium)

• Examples: Generative Adversarial Networks, multi-agent RL, PCA, off-policy evaluation, robust optimization, ...

Generative Adversarial Networks

$$\min_{G} \max_{D} f(D,G) = \mathbb{E}_{x \sim p_{\text{data}}} \left[\log(D(x)) \right] + \mathbb{E}_{z \sim p_z} \left[\log(1 - D(G(z))) \right]$$



Nash Equilibrium

$$\mathbf{z}_i^* \in \operatorname*{arg\,min}_{\mathbf{z}_i} f_i(\mathbf{z}_i, \mathbf{z}_{-i}^*)$$

THE PRISONER'S DILEMMA



Differentiable Games

• Differentiable games are much harder to solve (even only two-player)!

$\min_{\mathbf{x}} \max_{\mathbf{y}} f(\mathbf{x}, \mathbf{y})$

(It's called minimax optimization, saddle-point problem)

- Why are they more challenging?
 - In the nonconvex-nonconcave case, local Nash equilibria might not exist. Even when they exist, finding a local Nash equilibrium is PPAD-complete.
 - In the convex-concave setting, standard gradient descent can diverge with any positive step size or enter limit cycles.
 - Even when gradient descent converges, the rate of convergence may be too slow in practice (our focus today).



Left: bilinear game with f(x, y) = 10xyRight: $f(x, y) = 0.5x^2 + 10xy - 0.5y^2$

Today

• We are going to focus on two-player, strongly-convex strongly-concave, zero-sum games.

$$\min_{\mathbf{x}} \max_{\mathbf{y}} f(\mathbf{x}, \mathbf{y})$$

(many insights carry over to more general settings)



• Strong duality (minimax theorem) holds, i.e.,

$$\min_{\mathbf{x}} \max_{\mathbf{y}} f(\mathbf{x}, \mathbf{y}) = \max_{\mathbf{y}} \min_{\mathbf{x}} f(\mathbf{x}, \mathbf{y})$$

- Local Nash equilibrium is global and it is unique.
- Even for this simple setting, convergence can be slow because the "rotational force" necessitate extremely small learning rates.

A Closer Look of Linear Case

• Consider the general dynamics:

$$\mathbf{z}^{(k+1)} = \mathbf{z}^{(k)} - \eta F(\mathbf{z}^{(k)})$$

(where F is a vector field)

- Linear case: $F(\mathbf{z}) = \mathbf{H}\mathbf{z}$
 - Minimization: H is symmetric and all eigenvalues are real
 - **Differentiable Games: H** is non-symmetric and can have complex eigenvalues (with large imaginary parts)





 $\min_x \max_y f(x, y) = 0.5x^2 + 10xy - 0.5y^2$

Simultaneous Gradient Descent-Ascent

Simultaneous Gradient Descent-Ascent

• Sim-GDA is a naïve extension to gradient descent to the game setting

$$\begin{aligned} \mathbf{x}^{(k+1)} &\leftarrow \mathbf{x}^{(k)} - \eta \nabla_{\mathbf{x}} f(\mathbf{x}^{(k)}, \mathbf{y}^{(k)}) \\ \mathbf{y}^{(k+1)} &\leftarrow \mathbf{y}^{(k)} + \eta \nabla_{\mathbf{y}} f(\mathbf{x}^{(k)}, \mathbf{y}^{(k)}) \end{aligned}$$

- We can compactly write it as $\mathbf{z}^{(k+1)} \leftarrow \mathbf{z}^{(k)} \eta F(\mathbf{z}^{(k)})$ where $\mathbf{z} = [\mathbf{x}^{\top}, \mathbf{y}^{\top}]^{\top}$ and $F(\mathbf{z}) = [\nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{y})^{\top}, -\nabla_{\mathbf{y}} f(\mathbf{x}, \mathbf{y})^{\top}]^{\top}$.
- Assuming a quadratic problem $f(\mathbf{x}, \mathbf{y}) = \frac{1}{2}\mathbf{x}^{\top}\mathbf{A}\mathbf{x} + \mathbf{x}^{\top}\mathbf{B}\mathbf{y} \frac{1}{2}\mathbf{y}^{\top}\mathbf{C}\mathbf{y}$
 - We have the dynamics:

$$\mathbf{z}^{(k+1)} \leftarrow (\mathbf{I} - \eta \mathbf{H}) \mathbf{z}^{(k)}$$

where $\mathbf{z} = [\mathbf{x}^{\top}, \mathbf{y}^{\top}]^{\top}$ and $\mathbf{H} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^{\top} & \mathbf{C} \end{bmatrix}$

Convergence Analysis of Sim-GDA

- Setting: Smooth and strongly-monotone games
 - Define the gradient vector field $F(\mathbf{z}) = [\nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{y})^{\top}, -\nabla_{\mathbf{y}} f(\mathbf{x}, \mathbf{y})^{\top}]^{\top}$
 - Lipschitz Smooth: a vector field F is Lipschitz if for any $\mathbf{z}_1, \mathbf{z}_2$ and a parameter L:

$$||F(\mathbf{z}_1) - F(\mathbf{z}_2)|| \le L ||\mathbf{z}_1 - \mathbf{z}_2||$$

• Strongly Monotone: a vector field F is strongly monotone if for any $\mathbf{z}_1, \mathbf{z}_2$ and a parameter μ :

$$(F(\mathbf{z}_1) - F(\mathbf{z}_2))^{\top}(\mathbf{z}_1 - \mathbf{z}_2) \ge \mu \|\mathbf{z}_1 - \mathbf{z}_2\|^2$$

- Condition number: $\kappa \triangleq \frac{L}{\mu}$
- Quadratic case: $F(\mathbf{z}) = \mathbf{H}\mathbf{z}$ where $\mathbf{H} \succeq \mu \mathbf{I}$ and $\|\mathbf{H}\| \le L$

Convergence Analysis of Sim-GDA

- Recall that the dynamics of Sim-GDA: $\mathbf{z}^{(k+1)} \leftarrow (\mathbf{I} \eta \mathbf{H})\mathbf{z}^{(k)}$
- Its convergence rate is $\min_{\eta} \rho(\mathbf{I} \eta \mathbf{H}) = \min_{\eta} \max_{\lambda \in S_{\mathsf{D}}(\mathbf{H})} \|1 \eta \lambda\|$



Improved Game Dynamics



- The best convergence rate is limited by the eigenvalue $\lambda = \mu + \sqrt{L^2 - \mu^2}i.$
- The optimal convergence rate is $1 \frac{1}{\kappa^2}$, which implies that Sim-GDA takes roughly $\mathcal{O}(\kappa^2)$ steps to converge. Recall that gradient descent only takes $\mathcal{O}(\kappa)$ steps to converge in minimizing a strongly-convex function!

Could we accelerate the convergence of Sim-GDA?

Alternating Gradient Descent-Ascent

• Alt-GDA updates multiple players sequentially:

$$\begin{aligned} \mathbf{x}^{(k+1)} &\leftarrow \mathbf{x}^{(k)} - \eta \nabla_{\mathbf{x}} f(\mathbf{x}^{(k)}, \mathbf{y}^{(k)}) \\ \mathbf{y}^{(k+1)} &\leftarrow \mathbf{y}^{(k)} + \eta \nabla_{\mathbf{y}} f(\mathbf{x}^{(k+1)}, \mathbf{y}^{(k)}) \end{aligned}$$

- Alt-GDA converges with O(κ) steps (which matches the coarse lower-bound).
- The result could be extended to n-player setting (ongoing work).
- In the bilinear case, Alt-GDA is a symplectic integrator applied on the continuous dynamic.



Left: f(x, y) = 10xy;Right: $0.5x^2 + 10xy - 0.5y^2;$ Top: Sim-GDA; Bottem: Alt-GDA.

• The discussion of simultaneous and alternating updates dates back to the Jacobi and Gauss-Seidel methods in numerical linear algebra, see the celebrated Stein-Rosenberg theorem.

see more details in "Don't fix what ain't broke: near-optimal local convergence of alternating gradient descent-ascent for minimax optimization"

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Alternating Gradient Descent-Ascent

- Consider the quadratic problem $f(\mathbf{x}, \mathbf{y}) = \frac{1}{2}\mathbf{x}^{\top}\mathbf{A}\mathbf{x} + \mathbf{x}^{\top}\mathbf{B}\mathbf{y} \frac{1}{2}\mathbf{y}^{\top}\mathbf{C}\mathbf{y}$.
- We have Alt-GDA as the following form:

$$\begin{bmatrix} \mathbf{x}^{(k+1)} \\ \mathbf{y}^{(k+1)} \end{bmatrix} \leftarrow \underbrace{\begin{bmatrix} \mathbf{I} - \eta \mathbf{A} & -\eta \mathbf{B} \\ \eta \mathbf{B}^\top (\mathbf{I} - \eta \mathbf{A}) & \mathbf{I} - \eta \mathbf{C} - \eta^2 \mathbf{B}^\top \mathbf{B} \end{bmatrix}}_{\mathbf{J}_{\text{Alt}}} \begin{bmatrix} \mathbf{x}^{(k)} \\ \mathbf{y}^{(k)} \end{bmatrix}$$

• Recall Sim-GDA dynamcis for the quadratic case:

$$\begin{bmatrix} \mathbf{x}^{(k+1)} \\ \mathbf{y}^{(k+1)} \end{bmatrix} \leftarrow \underbrace{\begin{bmatrix} \mathbf{I} - \eta \mathbf{A} & -\eta \mathbf{B} \\ \eta \mathbf{B}^\top & \mathbf{I} - \eta \mathbf{C} \end{bmatrix}}_{\mathbf{J}_{\mathrm{Sim}}} \begin{bmatrix} \mathbf{x}^{(k)} \\ \mathbf{y}^{(k)} \end{bmatrix}$$

• Alt-GDA allows us to use **larger** step sizes. The optimal step size for Sim-GDA is $\frac{\mu}{L^2}$ while the optimal one for Alt-GDA is roughly $\frac{1}{L}$.



Eigenvalues of \mathbf{J}_{Alt} (green dots) and \mathbf{J}_{Sim} (red dots) for the minimax problem $f(x, y) = 0.3x^2 + 1.2xy - 0.3y^2$. Their trajectories as η sweeps in [0, 1] are shown from light colors to dark colors

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Alternating Gradient Descent-Ascent

• We are implicitly using alternating updates in GAN training.



DCGAN on CIFAR-10. Left: SGD as base optimizer; Right: AMSGrad as base optimizer.

Negative Momentum

• Negative momentum is basically Heavy-ball momentum with a negative damping value:

$$\mathbf{z}^{(k+1)} \leftarrow (1+\beta)\mathbf{z}^{(k)} - \beta\mathbf{z}^{(k-1)} - \eta F(\mathbf{z}^{(k)})$$

- Intuition: negative momentum reduces the imaginary parts of complex eigenvalues, and hence suppresses the rotational behaviour. (recall the rate of Sim-GDA was limited by the eigevalue $\lambda = \mu + \sqrt{L^2 \mu^2}i$)
- Negative momentum converges in $\mathcal{O}(\kappa^{1.5})$ steps, which is slightly faster than Sim-GDA (recall the complexity of $\mathcal{O}(\kappa^2)$). However, this rate is suboptimal as some other algorithms converge in $\mathcal{O}(\kappa)$ steps.
- Proving this convergence rate is extremely **hard**! Need to leverage the connection between Chebyshev polynomial and Heavy-ball momentum. Check out my paper "On the suboptimality of negative momentum for minimax optimization".

Negative Momentum

• Negative momentum is basically Heavy-ball momentum with a negative damping value:

$$\mathbf{z}^{(k+1)} \leftarrow (1+\beta)\mathbf{z}^{(k)} - \beta \mathbf{z}^{(k-1)} - \eta F(\mathbf{z}^{(k)})$$

- Fact: Heavy-ball momentum with an optimally-tuned damping parameter is optimal when all eigenvalues of **H** fall within an ellipse in the complex plane.
- $\frac{(\Re \lambda d)^2}{a^2} + \frac{(\Im \lambda)^2}{b^2} \le 1$ a > b: optimal β is positive • a < b: optimal β is negative • a = b: optimal β is zero
- Another fun fact: Negative momentum retains the same convergence rate when the function f is not quadratic. (Recall that Heavy-ball momentum only achieves acceleration when f is quadratic)

see more details in "Don't fix what ain't broke: near-optimal local convergence of alternating gradient descent-ascent for minimax optimization"

Negative Momentum



Image Credit: Negative Momentum for Improved Game Dynamics

Proximal Point Method

• The proximal point method (Rockafeller, 1976) is an implicit method:

$$\mathbf{z}^{(k+1)} \leftarrow \mathbf{z}^{(k)} - \eta F(\mathbf{z}^{(k+1)})$$

- Intuition: compute gradient at a future point, but it is not implementable in many cases (chicken and egg situtation).
- In optimization, the proximal point method is largely regarded as a "conceptual" guiding principle for accelerating optimization algorithms. NAG can be derived from the proximal point method (see "From Proximal Point Method to Nesterov's Acceleration" paper).
- It can be shown that for smooth and strongly monotone games, the proximal point method converges linearly for any η:

$$\|\mathbf{z}^{(k)} - \mathbf{z}^*\|^2 \le \left(\frac{1}{1+2\eta\mu}\right)^k \|\mathbf{z}^{(0)} - \mathbf{z}^*\|^2$$

check out the proof in "A Unified Analysis of First-Order Methods for Smooth Games via Integral Quadratic Constraints"

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Could we approximate proximal point method and achieve acceleration?

Extra-gradient method

• The Extra-gradient method computes the gradient with one-step lookahead (extrapolated gradient):

$$\mathbf{z}^{(k+1/2)} \leftarrow \mathbf{z}^{(k)} - \eta F(\mathbf{z}^{(k)})$$
$$\mathbf{z}^{(k+1)} \leftarrow \mathbf{z}^{(k)} - \eta F(\mathbf{z}^{(k+1/2)})$$

- It was first proposed by Korpelevich in 70's to solve monotone variational inequality problem.
- It was recently re-introduced by Gidel, et.al (2019) and Mokhtari, et.al (2019) in the context of differentiable games and minimax optimization.
- Over the last three years, more than 10 papers discussed the extra-gradient method in different settings.

Extra-gradient method

• The extra-gradient method computes the gradient with one-step lookahead:

$$\mathbf{z}^{(k+1/2)} \leftarrow \mathbf{z}^{(k)} - \eta F(\mathbf{z}^{(k)})$$
$$\mathbf{z}^{(k+1)} \leftarrow \mathbf{z}^{(k)} - \eta F(\mathbf{z}^{(k+1/2)})$$

- Intuition: approximate $F(\mathbf{z}^{(k+1)})$ with $F(\mathbf{z}^{(k+1/2)})$, hoping to inherit the convergence properties of proximal point method.
- Formally, it can shown that starting with the same $\mathbf{z}^{(k)}$, the solution of extra-gradient $\mathbf{z}_{eg}^{(k+1)}$ after one step is relatively close to the solution of proximal point method $\mathbf{z}_{ppm}^{(k+1)}$:

$$\|\mathbf{z}_{eg}^{(k+1)} - \mathbf{z}_{ppm}^{(k+1)}\| \le o(\eta^2)$$

• Under the same set of assumptions, the extra-gradient method converges linearly

$$\|\mathbf{z}^{(k)} - \mathbf{z}^*\|^2 \le \left(1 - \frac{1}{2\kappa}\right)^k \|\mathbf{z}^{(0)} - \mathbf{z}^*\|^2$$

see more details in "A Unified Analysis of Extra-gradient and Optimistic Gradient Methods for Saddle Point Problems: Proximal Point Approach"

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Optimistic Gradient Method

• Optimistic Gradient update rule:

$$\mathbf{z}^{(k+1)} \leftarrow \mathbf{z}^{(k)} - \eta F(2\mathbf{z}^{(k)} - \mathbf{z}^{(k-1)})$$

• You could understand it as replacing the first step of extra-gradient with the following:

$$\mathbf{z}^{(k+1/2)} \leftarrow \mathbf{z}^{(k)} + \mathbf{z}^{(k)} - \mathbf{z}^{(k-1)}$$

- It has pretty much the same convergence properties as extra-gradient but only compute the gradient once in every iteration!
- Under the same set of assumptions, optimistic gradient converges linearly

$$\|\mathbf{z}^{(k)} - \mathbf{z}^*\|^2 \le \left(1 - \frac{1}{4\kappa}\right)^k \|\mathbf{z}^{(0)} - \mathbf{z}^*\|^2$$

- In which case should we use optimistic gradient method?
 - In the situation that you are only allowed to query the gradient once every iteration.
 - In (no-regret) online learning with an arbitrary adversary, extra-gradient is not *no-regret*.

Comparison between different algorithms



Distances to the optimum as a function of iterations on a quadratic minimax problem.

Important directions that I didn't cover

- General convex-concave setting (without strong convexity/concavity). In this setting, one can only achieve sublinear convergence (see e.g., [1,2]).
- Stochastic settings (see e.g., [3, 4]).
- Second-order methods (see e.g., [5, 6]).
- Sequential games when f is nonconvex-nonconcave (see e.g., [7, 8]). In this case, Nash equilibrium might not exist and other equilibrium concepts were proposed. Moreover, the order of different players matters since min max \neq max min

[1] Convergence rate of o(1/k) for optimistic gradient and extragradient methods in smooth convex-concave saddle point problems.

[2] Last iterate is slower than averaged iterate in smooth convex-concave saddle point problems.

[3] On the convergence of single-call stochastic extragradient methods.

[4] Explore Aggressively, Update Conservatively: Stochastic Extragradient Methods with Variable Stepsize Scaling.

[5] Differentiable Game Mechanics.

- [6] Competitive Gradient Descent.
- [7] What is Local Optimality in Nonconvex-Nonconcave Minimax Optimization?
- [8] On Solving Minimax Optimization Locally: A Follow-the-Ridge Approach.

Summary

- Differentiable game dynamics is more complex.
- In the nonconvex setting, Nash equilibrium might not exist. Even when it exists, finding local solution is much harder than finding local minima in minimization.
- Even for convex-concave two-player setting, standard algorithms could either diverge or cycle around the equilibrium.
- When converges, rotational component (caused by complex eigenvalues) would slow down convergence.
- When it comes to algorithm choice, alternating updates significantly outperform simultaneous updates and negative momentum is preferred in many cases.
- Extra-gradient and optimistic gradient method approximate proximal point method, which accelerate the convergence.