How to Escape Saddle Points Efficiently?

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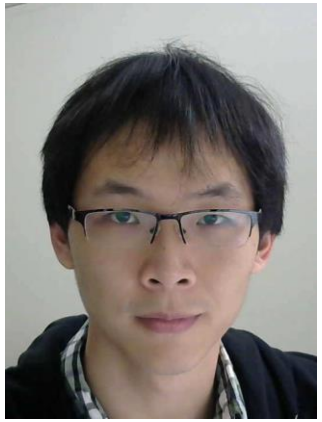

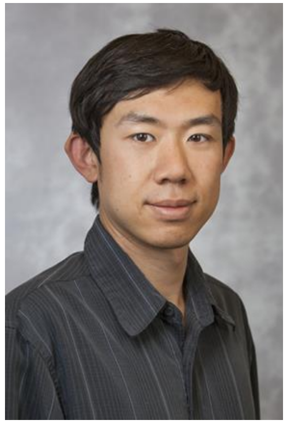


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Duke Univ.

Sham M. Kakade
U Washington

Nonconvex optimization

Problem: $\min_{x} f(x)$ $f(\cdot)$: nonconvex function

Applications: Deep learning, compressed sensing, matrix completion, dictionary learning, nonnegative matrix factorization, …

Gradient descent (GD) [Cauchy 1847]

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

Question

How does it perform?

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How does it perform?

<u>Answer</u>

Converges to first order stationary points

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How does it perform?

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Definition

ϵ-First order stationary point (ϵ-FOSP) : $\|\nabla f(x)\| \leq \epsilon$

Gradient descent (GD) [Cauchy 1847]

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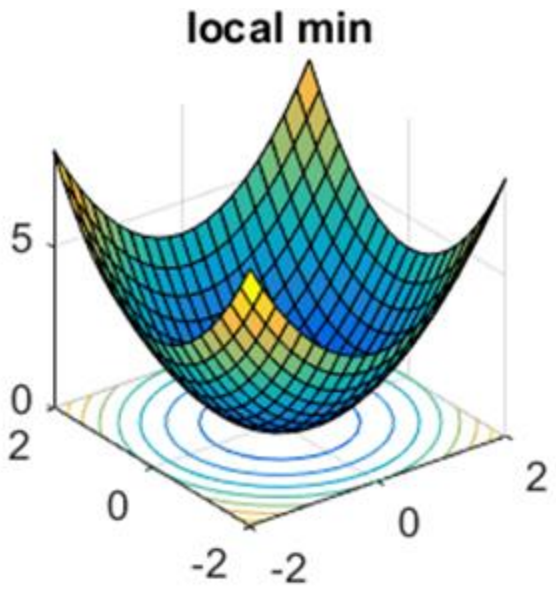
Question
How does it perform?

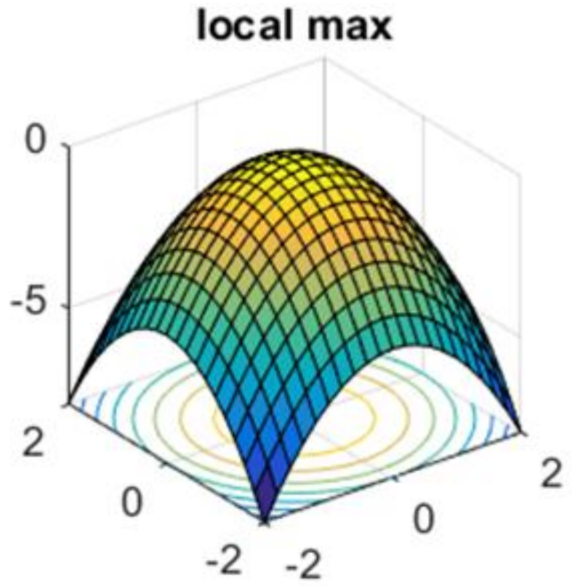
Answer
Converges to first order stationary points

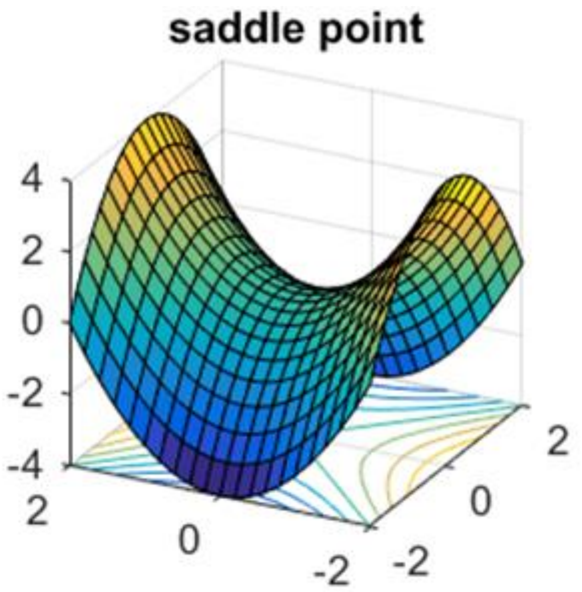
Definition
ϵ-First order stationary point (ϵ-FOSP) : $\|\nabla f(x)\| \leq \epsilon$

Concretely
ϵ-FOSP in $O\left(\frac{1}{\epsilon^2}\right)$ iterations
[Folklore]

How do FOSPs look like?







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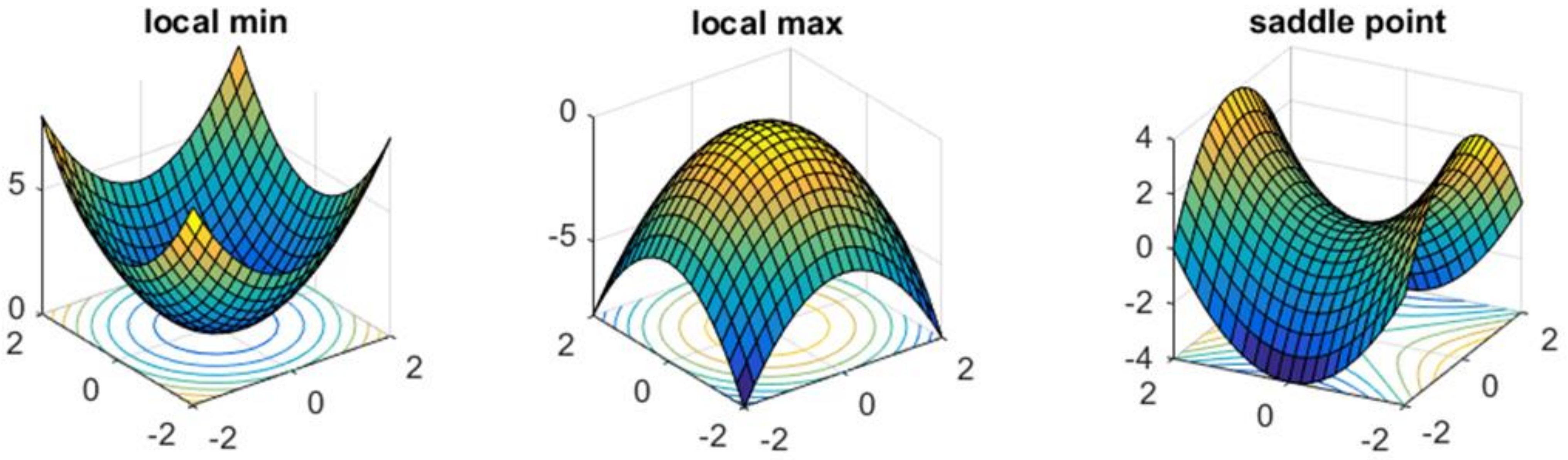
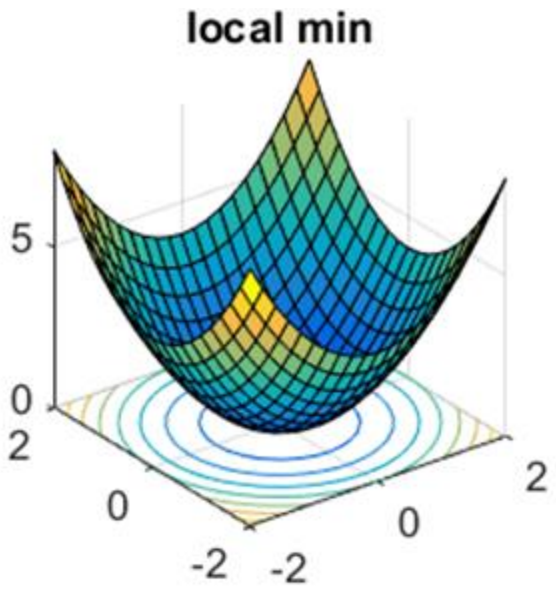


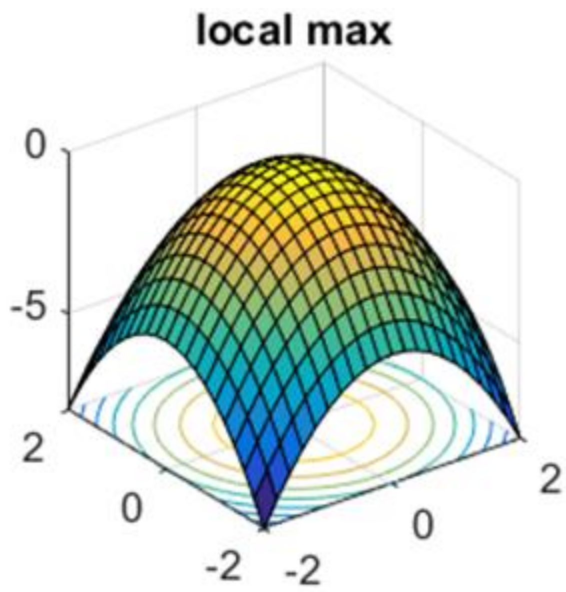
Hessian PSD

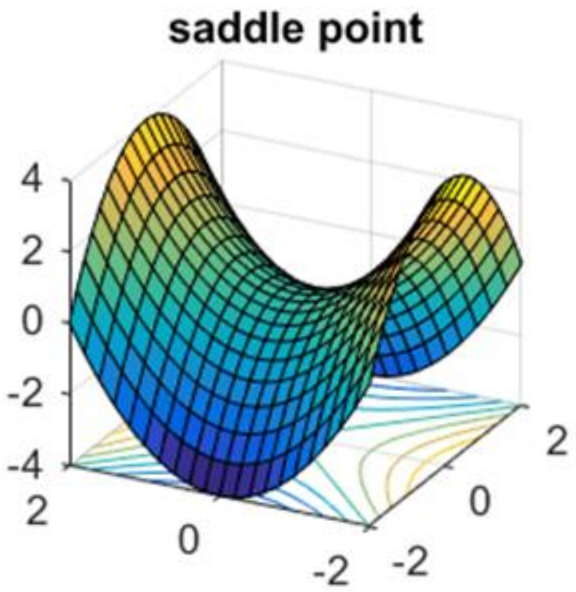
$\nabla^2 f(x) \succcurlyeq 0$

Second order stationary points (SOSP)

How do FOSPs look like?







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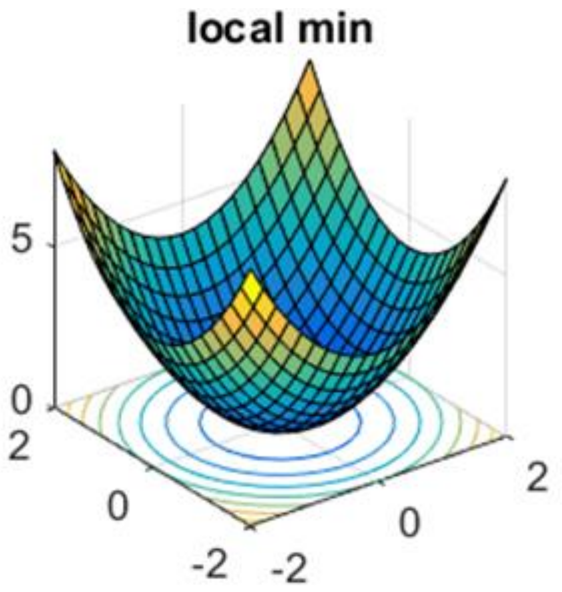

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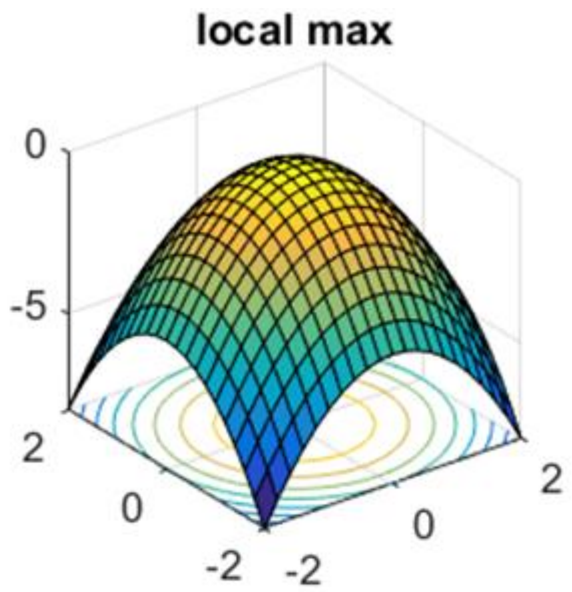
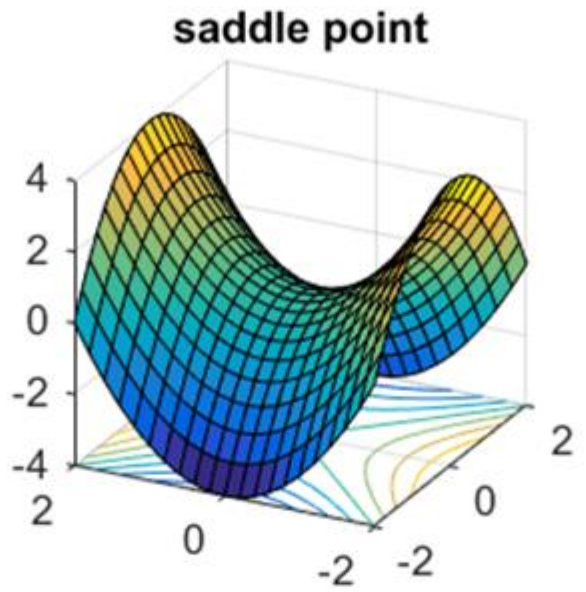
Second order stationary points (SOSP)



Hessian NSD

$\nabla^2 f(x) \preccurlyeq 0$



Hessian indefinite

$\lambda_{\min}(\nabla^2 f(x)) \leq 0$

$\lambda_{\max}(\nabla^2 f(x)) \geq 0$

FOSPs in popular problems

- Very well studied
  - Neural networks [Dauphin et al. 2014]
  - Matrix sensing [Bhojanapalli et al. 2016]
  - Matrix completion [Ge et al. 2016]
  - Robust PCA [Ge et al. 2017]
  - Tensor factorization [Ge et al. 2015, Ge & Ma 2017]
  - Smooth semidefinite programs [Boumal et al. 2016]
  - Synchronization & community detection [Bandeira et al. 2016, Mei et al. 2017]

Two major observations

- FOSPs: proliferation (exponential #) of saddle points
  - Recall FOSP $\triangleq \nabla f(x) = 0$
  - Gradient descent can get stuck near them
- SOSPs: not just local minima; as good as global minima
  - Recall SOSP $\triangleq \nabla f(x) = 0$ & $\nabla^2 f(x) \succcurlyeq 0$

<u>Upshot</u>

1. FOSP not good enough
2. Finding SOSP sufficient

Can gradient descent find SOSPs?

- Yes, perturbed GD finds an ϵ-SOSP in $O\left(\text{poly}\left(\frac{d}{\epsilon}\right)\right)$ iterations [Ge et al. 2015]

- GD is a first order method while SOSP captures second order information

Can gradient descent find SOSPs?

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<u>Question 1</u>

Does perturbed GD converge to SOSP **efficiently**?
In particular, **independent of $\boldsymbol{d}$**?

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<u>Question 1</u>

Does perturbed GD converge to SOSP **efficiently**?

In particular, **independent of $\boldsymbol{d}$**?

<u>Our result</u>

Almost yes, in $\tilde{O}\left(\frac{\mathrm{polylog}(d)}{\epsilon^2}\right)$ iterations!

Accelerated gradient descent (AGD) [Nesterov 1983]

- Optimal algorithm in the convex setting
- Practice: Sutskever et al. 2013 observed AGD to be much faster than GD
- Widely used in training neural networks since then
- Theory: Finds an ϵ-FOSP in $O\left(\frac{1}{\epsilon^2}\right)$ iterations [Ghadimi & Lan 2013]
- No improvement over GD

Question 2: Does essentially pure AGD find SOSPs faster than GD?

- Our result: Yes, in $\tilde{O}\left(\frac{\mathrm{polylog}(d)}{\epsilon^{1.75}}\right)$ steps compared to $\tilde{O}\left(\frac{\mathrm{polylog}(d)}{\epsilon^{2}}\right)$ for GD

- Perturbation + negative curvature exploitation (NCE) on top of AGD
  - NCE inspired by Carmon et al. 2017

- Carmon et al. 2016 and Agarwal et al. 2017 show this improved rate for a more complicated algorithm
  - Solve sequence of regularized problems using AGD

Summary

ϵ-SOSP [Nesterov & Polyak 2006]

$\|\nabla f(x)\| \leq \epsilon$ & $\lambda_{\min}(\nabla^2 f(x)) \gtrsim -\sqrt{\epsilon}$

- Convergence to SOSPs very important in practice
- Pure GD and AGD can get stuck near FOSPs (saddle points)

Algorithm	Paper	# Iterations	Simplicity
Perturbed gradient descent	Ge et al. 2015 Levy 2016	$O\left(\text{poly}\left(\frac{d}{\epsilon}\right)\right)$	Single loop
	Jin, Ge, N., Kakade, Jordan 2017	$\boldsymbol{\tilde{O}\left(\frac{\text{polylog}(d)}{\epsilon^2}\right)}$	**Single loop**
Sequence of regularized subproblems with AGD	Carmon et al. 2016 Agarwal et al. 2017	$\tilde{O}\left(\frac{\text{polylog}(d)}{\epsilon^{1.75}}\right)$	Nested loop
Perturbed AGD + NCE	**Jin, N., Jordan 2017**	$\boldsymbol{\tilde{O}\left(\frac{\text{polylog}(d)}{\epsilon^{1.75}}\right)}$	**Single loop**

Part I

Main Ideas of the Proof of Gradient Descent

Setting

- **Gradient Lipschitz**: $\|\nabla f(x) - \nabla f(y)\| \lesssim \|x - y\|$

- **Hessian Lipschitz**: $\|\nabla^2 f(x) - \nabla^2 f(y)\| \lesssim \|x - y\|$

- **Lower bounded**: $\min_x f(x) > -\infty$

How does GD behave?

GD step

$x_{t+1} \leftarrow x_t - \eta \nabla f(x_t)$

Recall

FOSP: $\nabla f(x)$ small

SOSP: $\nabla f(x)$ small &
$\lambda_{\min}\left(\nabla^2 f(x)\right) \gtrsim 0$

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GD step
$x_{t+1} \leftarrow x_t - \eta \nabla f(x_t)$

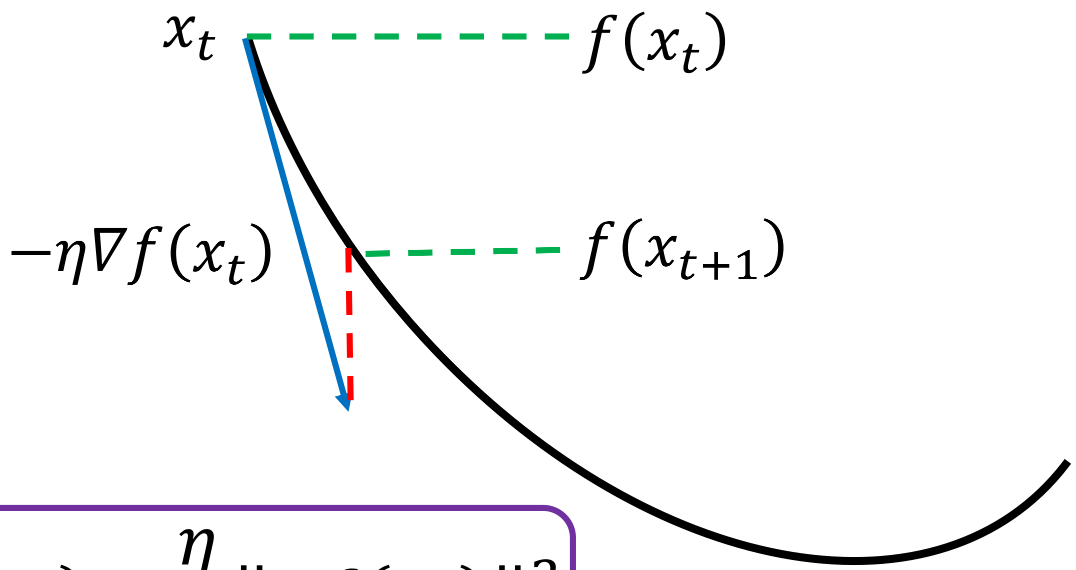
$\|\nabla f(x_t)\|$ small

SOSP

Saddle point

$\|\nabla f(x_t)\|$ large

$$f(x_{t+1}) \leq f(x_t) - \frac{\eta}{2}\|\nabla f(x_t)\|^2$$



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SOSP

Saddle point

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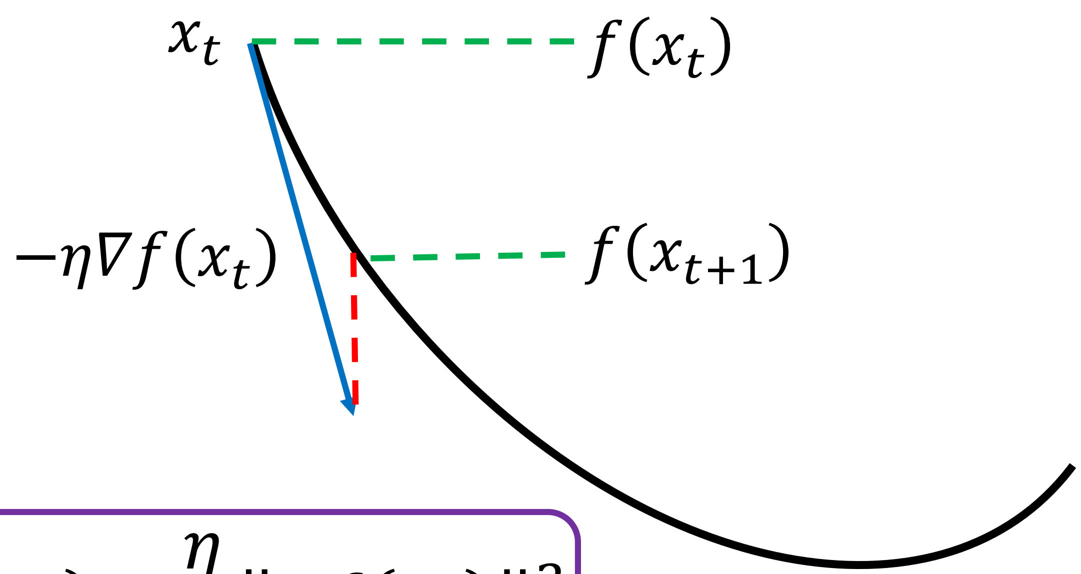
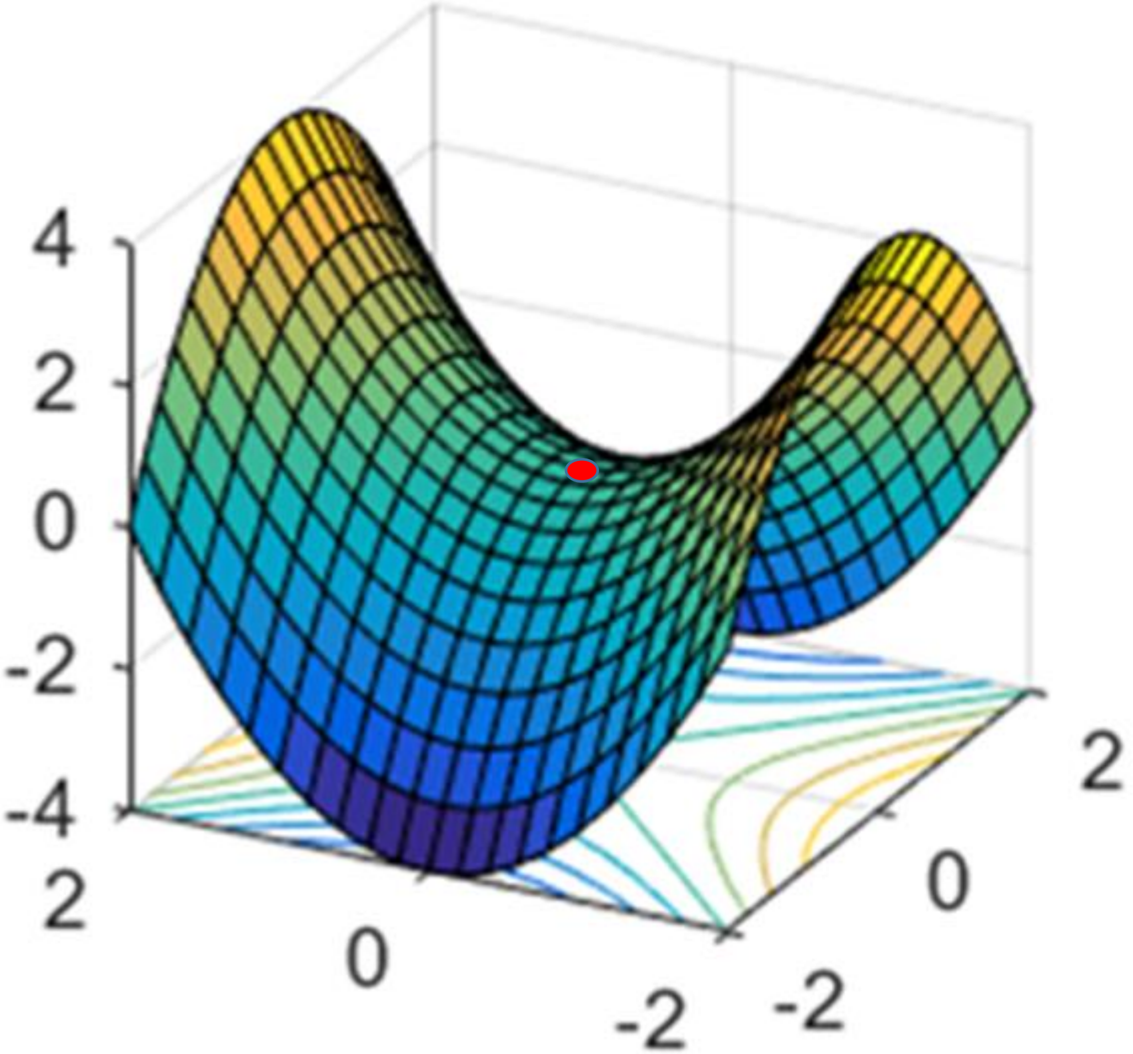


How to escape saddle points?



Perturbed gradient descent

1. **For** $t = 0,1,\cdots$ **do**
2. **if** perturbation_condition_holds **then**
3. $x_t \leftarrow x_t + \xi_t$ where $\xi_t \sim Unif\left(B_0(\epsilon)\right)$
4. $x_{t+1} \leftarrow x_t - \eta \nabla f(x_t)$

Perturbed gradient descent

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Between two perturbations, just run GD!

Perturbed gradient descent

1. $\nabla f(x_t)$ is small
2. No perturbation in last several iterations

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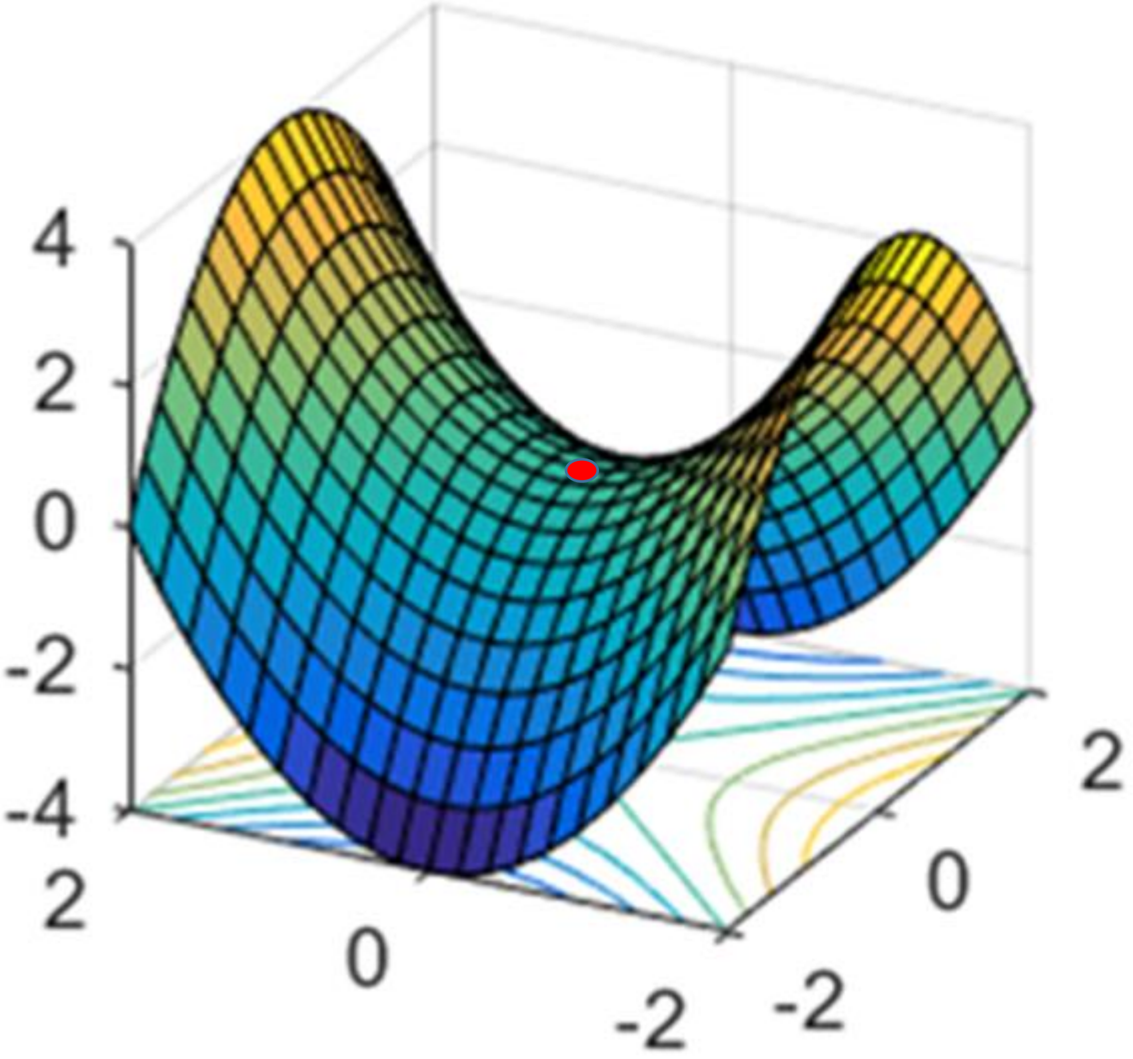
Between two perturbations, just run GD!

How can perturbation help?

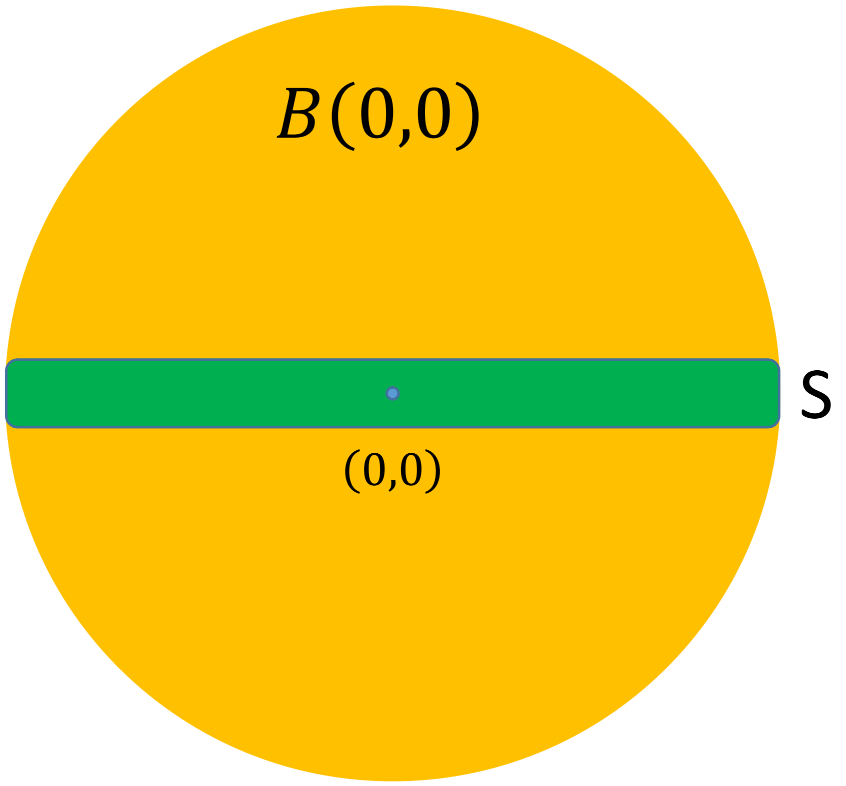


Key question

- $S \stackrel{\text{def}}{=}$ set of points around saddle point from where gradient descent does not escape quickly
- Escape $\stackrel{\text{def}}{=}$ function value decreases significantly
- How much is $\mathrm{Vol}(S)$?
- $\mathrm{Vol}(S)$ small $\Rightarrow$ perturbed GD escapes saddle points efficiently

Two dimensional quadratic case

- $f(x) = \frac{1}{2} x^\top \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} x$
- $\lambda_{\min}(H) = -1 < 0$
- $(0,0)$ is a saddle point
- GD: $x_{t+1} = \begin{bmatrix} 1-\eta & 0 \\ 0 & 1+\eta \end{bmatrix} x_t$
- S is a thin strip, $\mathrm{Vol}(S)$ is small



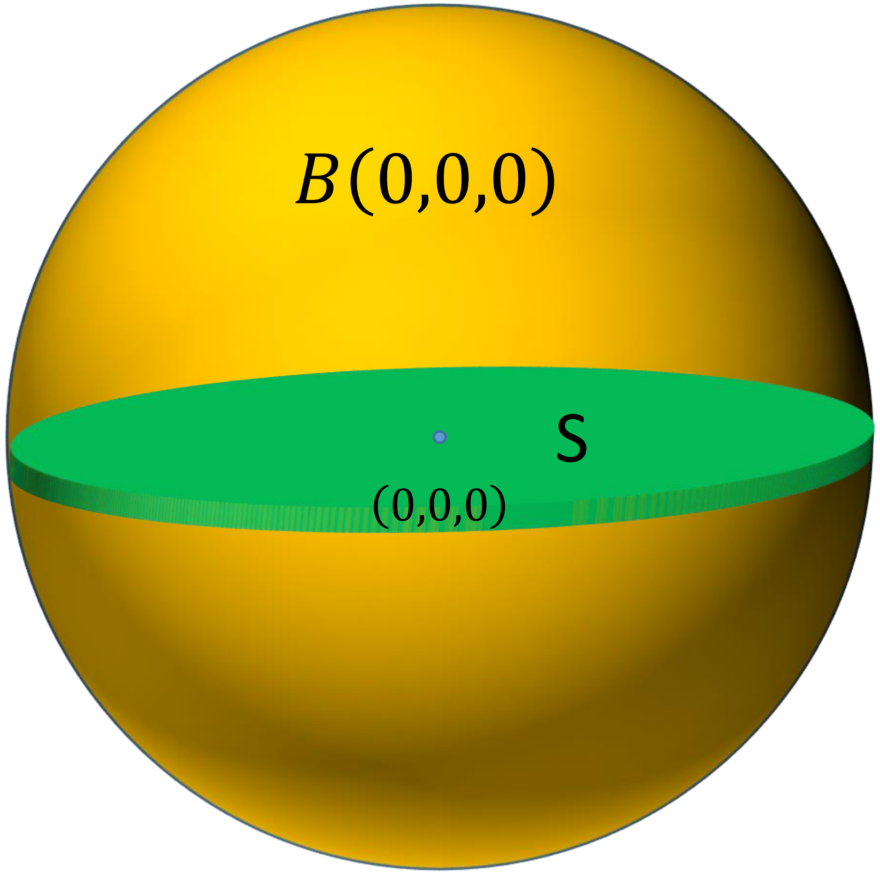
Three dimensional quadratic case

- $f(x) = \frac{1}{2} x^\top \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} x$

- $(0,0,0)$ is a saddle point

- GD: $x_{t+1} = \begin{bmatrix} 1-\eta & 0 & 0 \\ 0 & 1-\eta & 0 \\ 0 & 0 & 1+\eta \end{bmatrix} x_t$

- S is a thin disc, $\mathrm{Vol}(S)$ is small

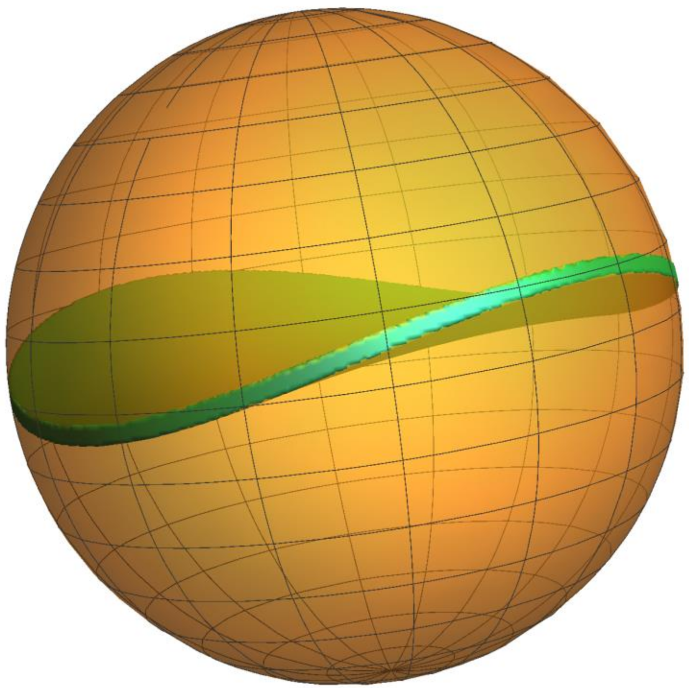


General case

Key technical results

S ~ thin deformed disc

$\mathrm{Vol}(S)$ is small



Two key ingredients of the proof

Improve or localize

$$f(x_{t+1}) \leq f(x_t) - \frac{\eta}{2} \|\nabla f(x_t)\|^2$$
$$= f(x_t) - \frac{\eta}{2} \left\| \frac{x_t - x_{t+1}}{\eta} \right\|^2$$

$$\|x_t - x_{t+1}\|^2 \leq 2\eta(f(x_t) - f(x_{t+1}))$$

$$\|x_0 - x_t\|^2 \leq t \sum_{i=0}^{t-1} \|x_i - x_{i+1}\|^2 \leq 2\eta t\big(f(x_0) - f(x_t)\big)$$

Two key ingredients of the proof

Improve or localize

Upshot

Either function value decreases significantly

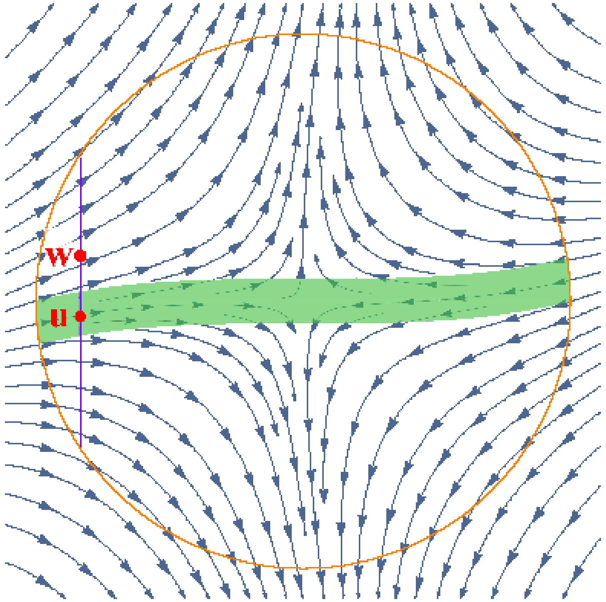
or iterates do not move much

$$\|x_0 - x_t\|^2 \le t \sum_{i=0}^{t-1} \|x_i - x_{i+1}\|^2 \le 2\eta t\big(f(x_0) - f(x_t)\big)$$

Proof idea

- If GD from either u or w goes outside a small ball, it escapes (function value ⬇)
- If GD from both u and w lie in a small ball, use local quadratic approximation of $f(\cdot)$
- Show the claim for exact quadratic, and bound approximation error using Hessian Lipschitz property

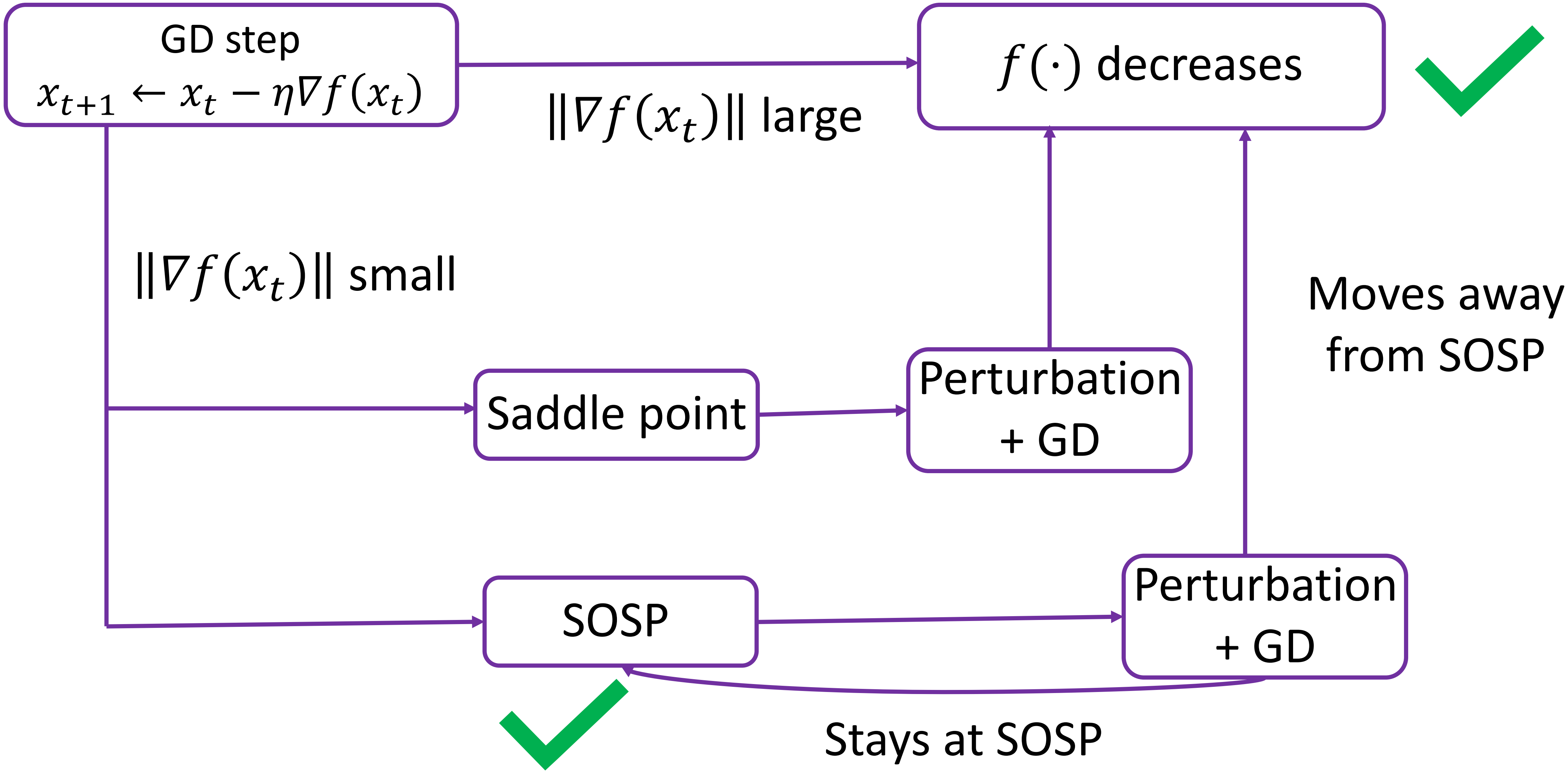
<u>Coupling</u>



Either GD from u escapes

Or GD from w escapes

Putting everything together



Part II

Main Ideas of the Proof of Accelerated Gradient Descent

Nesterov's AGD

Iterate x_t & Velocity v_t

1. $x_{t+1} = (x_t + (1-\theta)v_t) - \eta\nabla f(x_t + (1-\theta)v_t)$
2. $v_{t+1} = x_{t+1} - x_t$

Gradient descent at $x_t + (1-\theta)v_t$

<u>Challenge</u>

Known potential functions depend on optimum x^*

Differential equation view of AGD

- AGD is a discretization of the following ODE [Su et al. 2015]

$$\ddot{x} + \tilde{\theta}\dot{x} + \nabla f(x) = 0$$

- Multiplying by $\dot{x}$ and integrating from t_1 to t_2 gives us

$$f(x_{t_2}) + \frac{1}{2}\|\dot{x}_{t_2}\|^2 = f(x_{t_1}) + \frac{1}{2}\|\dot{x}_{t_1}\|^2 - \tilde{\theta}\int_{t_1}^{t_2}\|\dot{x}_t\|^2 dt$$

- Hamiltonian $f(x_t) + \frac{1}{2}\|\dot{x}_t\|^2$ decreases monotonically

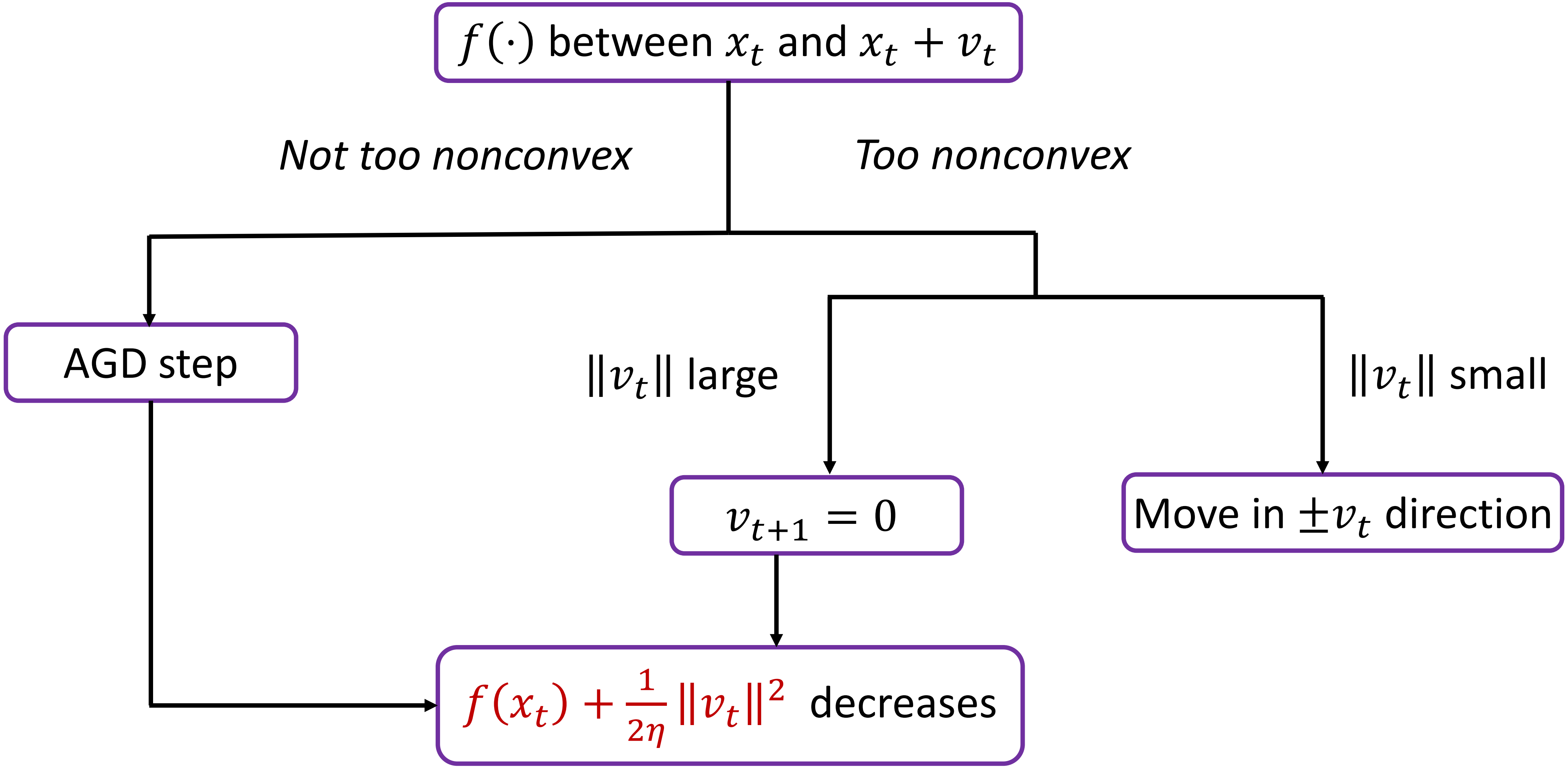
After discretization

Iterate: x_t and velocity: $v_t := x_t - x_{t-1}$

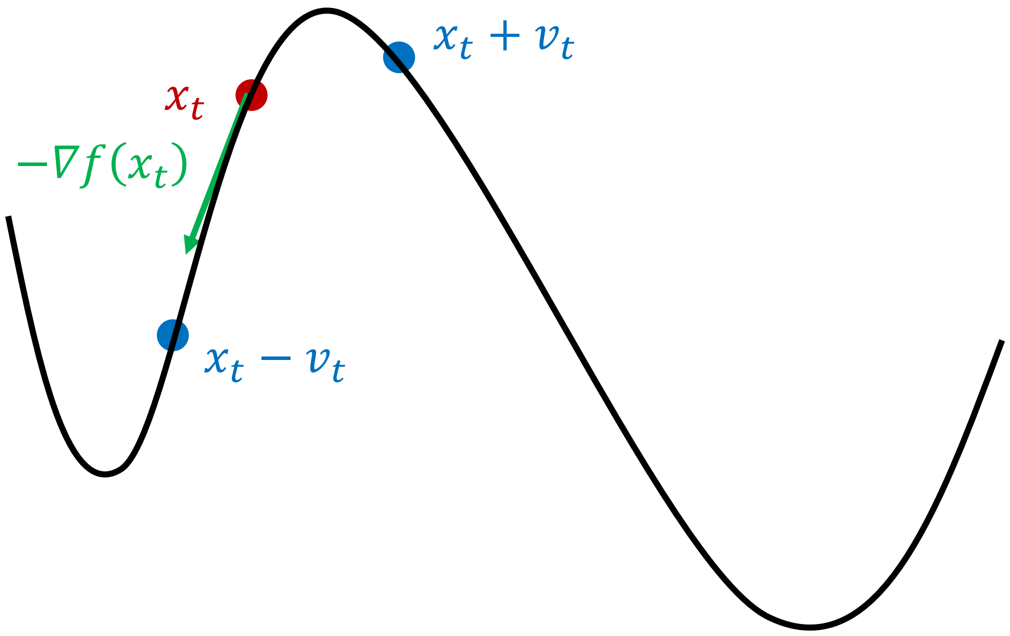
- Hamiltonian $f(x_t) + \frac{1}{2\eta}\|v_t\|^2$ decreases monotonically if $f(\cdot)$ *"not too nonconvex"* between x_t and $x_t + v_t$
  - *too nonconvex* = *negative curvature*
  - Can increase if $f(\cdot)$ is *"too nonconvex"*

- If the function is *"too nonconvex"*, reset velocity or move in nonconvex direction – *negative curvature exploitation*

Hamiltonian decrease

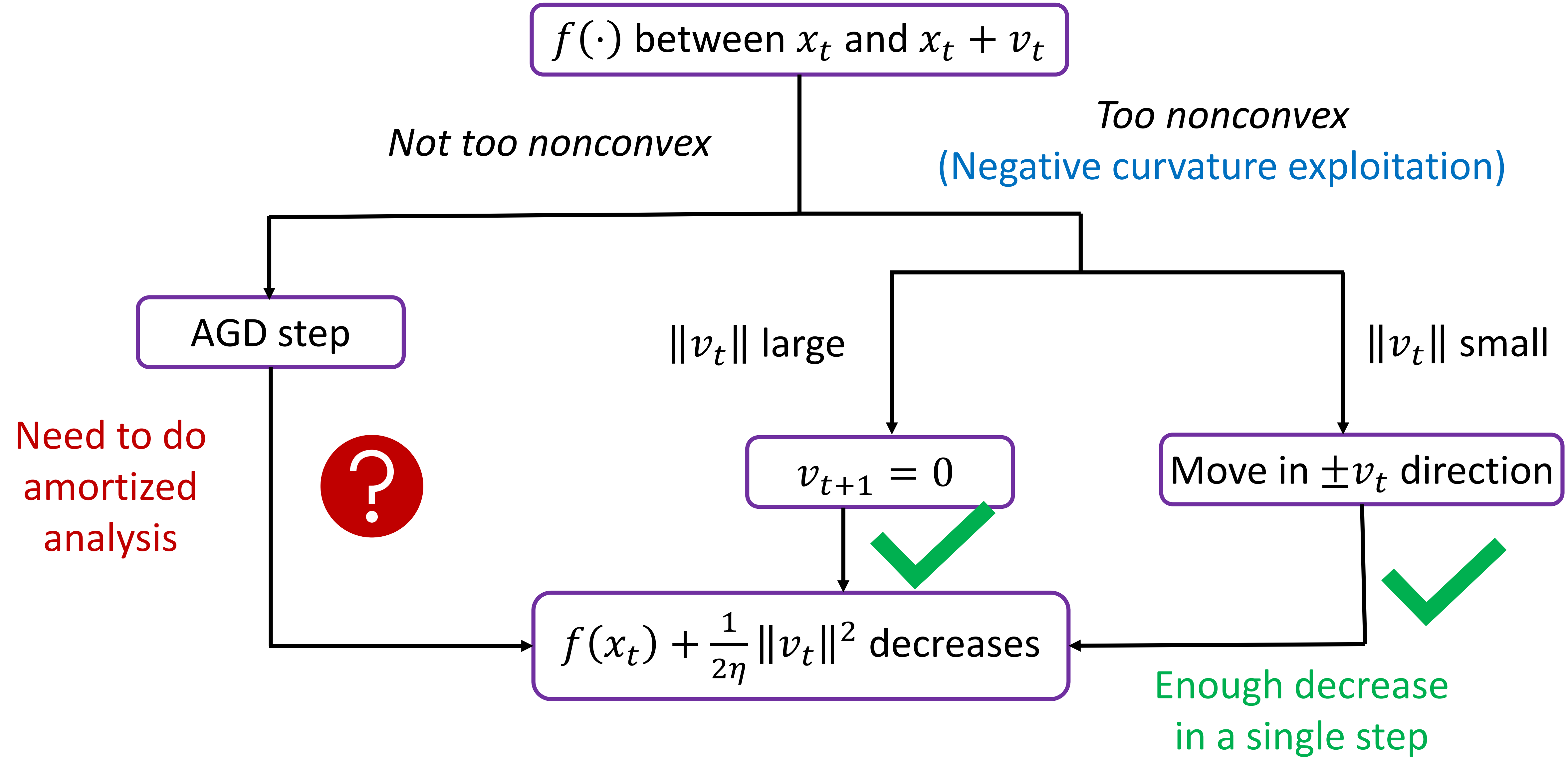


Negative curvature exploitation – $\|v_t\|$ small



One of $\pm v_t$ directions decreases $f(x_t)$

Hamiltonian decrease



Improve or localize

$$f(x_{t+1}) + \frac{1}{2\eta}\|v_{t+1}\|^2 \leq f(x_t) + \frac{1}{2\eta}\|v_t\|^2 - \frac{\theta}{2\eta}\|v_t\|^2$$

$$\sum_{t=0}^{T-1}\|x_{t+1} - x_t\|^2 \leq \frac{2\eta}{\theta} \cdot (f(x_0) - f(x_T))$$

- Approximate locally by a quadratic and perform computations
  - Precise computations are technically challenging

Summary

- Simple variations to GD/AGD ensure efficient escape from saddle points

- Fine understanding of geometric structure around saddle points

- Novel techniques of independent interest

- Some extensions to stochastic setting

Open questions

- Is NCE really necessary?
- Lower bounds – recent work by Carmon et al. 2017, but gaps between upper and lower bounds
- Extensions to stochastic setting
- Nonconvex optimization for faster algorithms

Thank you!

Questions?