Deep Learning + Reinforcement Learning
SUMMER SCHOOL

ÉCOLE D'ÉTÉ SUR
l'apprentissage profond + l'apprentissage par renforcement

Introduction to Optimization - Theory & Practice

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Introduction

- 1st paragraph of CIFAR e-mail:
  - I am writing … to invite you to deliver the lecture on "Introduction to Optimization – Theory & Practice".
- My reply after reading first paragraph:
  - Yup, happy to do it!
- 3rd (unread) paragraph of CIFAR e-mail:
  - This year, we are asking all of our speakers to provide a **45 minute** lecture.
- Me after looking later reading full invite:
  - "How do I possibly cover optimization theory *and* practice in 45 minutes?"

Real Introduction

- I am assuming you have already trained a deep learning model.
  - Probably using stochastic gradient descent (SGD) or a variant like Adam.
- And it might useful if I could answer questions like these:
  - Question 1: How do I set the step size?
  - Question 2: How I pick the mini-batch size?
  - Question 3: Should I use variance reduction?
  - Question 4: What about random shuffling?
  - Question 5: Should I use importance sampling?
  - Question 6: Are there faster algorithms?
  - Question 7: Should we just use Adam?

Disclaimer

- These questions are complicated, depending on many factors.
- I will just focus on applying SGD to differentiable functions.
  - And I will assume the basic setting of IID data (no reinforcement learning).
- I will overview some important trade-offs to consider in this setting.
  - Which may help improve your understanding of these questions.
  - I will necessarily need to skip over a lot of precise details.
- If you want to see the long/detailed version, see here:
  - https://www.cs.ubc.ca/~schmidtm/Courses/5XX-S22 (in progress, 6 hours in).
  - https://www.cs.ubc.ca/~schmidtm/Courses/5XX-S20 (old version).

Optimization and Gradient Descent

- We usually "train" models by solving an optimization problem.

$$\min_{w \in \mathbb{R}^d} f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

  - We have 'd' parameters 'w' that we can modify the fit the data better.
    - For a deep neural network, this would contain the parameters of the various layers.
  - We have a function 'f' that measures how well we fit the data.
    - Usually this function is the average over a set of 'n' functions f_i.
    - Each f_i measures how well we fit training example 'i'.
      - Could be squared error or cross entropy of network's predictions.

- Most popular DL algorithm is stochastic gradient descent (SGD).

Deterministic and Stochastic Gradient Descent

- For minimizing functions of the form:

$$f(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w)$$

- Deterministic gradient descent repeats the iteration:

$$w_{k+1} = w_k - \alpha_k \nabla f(w_k)$$

  - For a "step size" α_k.

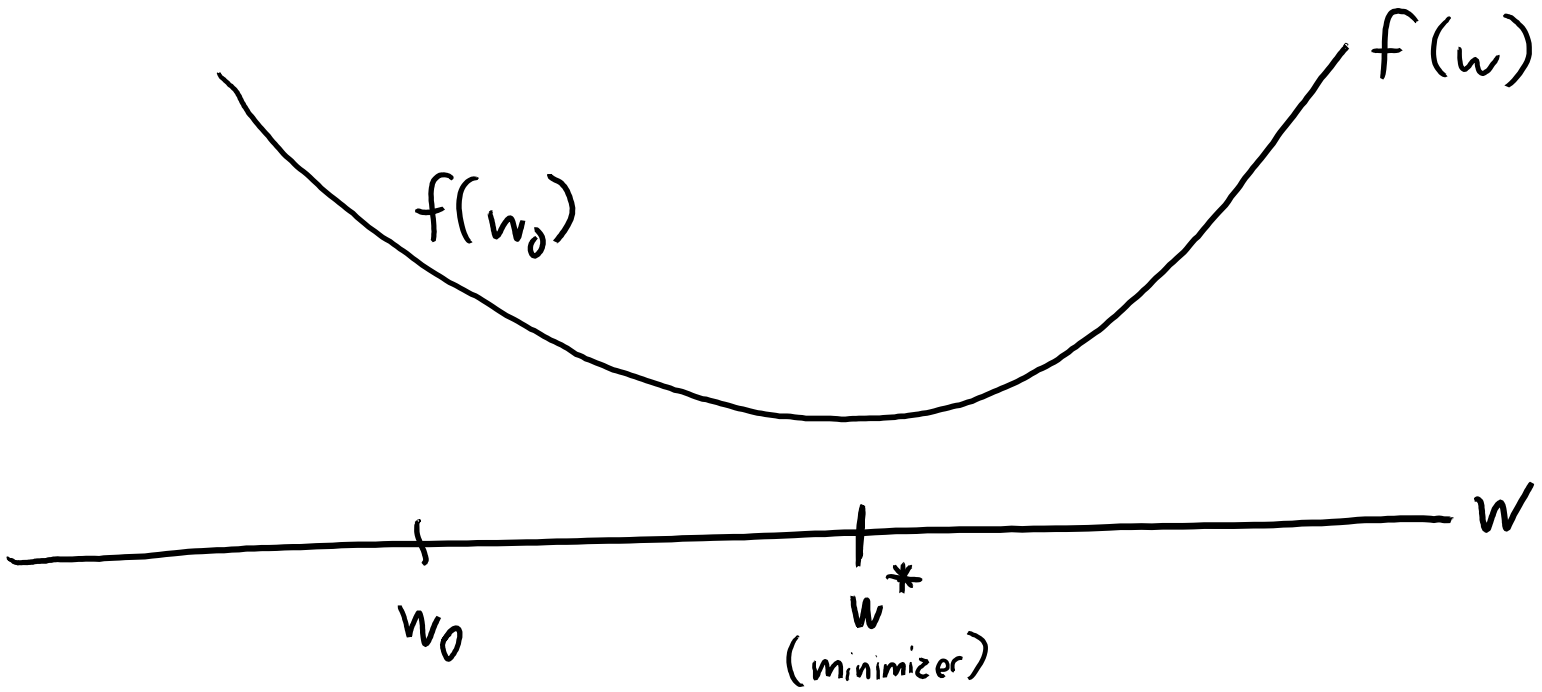
- Stochastic gradient descent repeats the iteration:

$$w_{k+1} = w_k - \alpha_k \nabla f_{i_k}(w_k)$$

  - For a random training example 'i_k'.
  - Key advantage is cost per iteration: 1 billion times faster for 1 billion examples.

Deterministic Gradient Descent in 1 Dimension

- Deterministic gradient descent is based on a simple observation:
  - Give parameters ‘w’, the direction of largest decrease is $-\nabla f(w)$.



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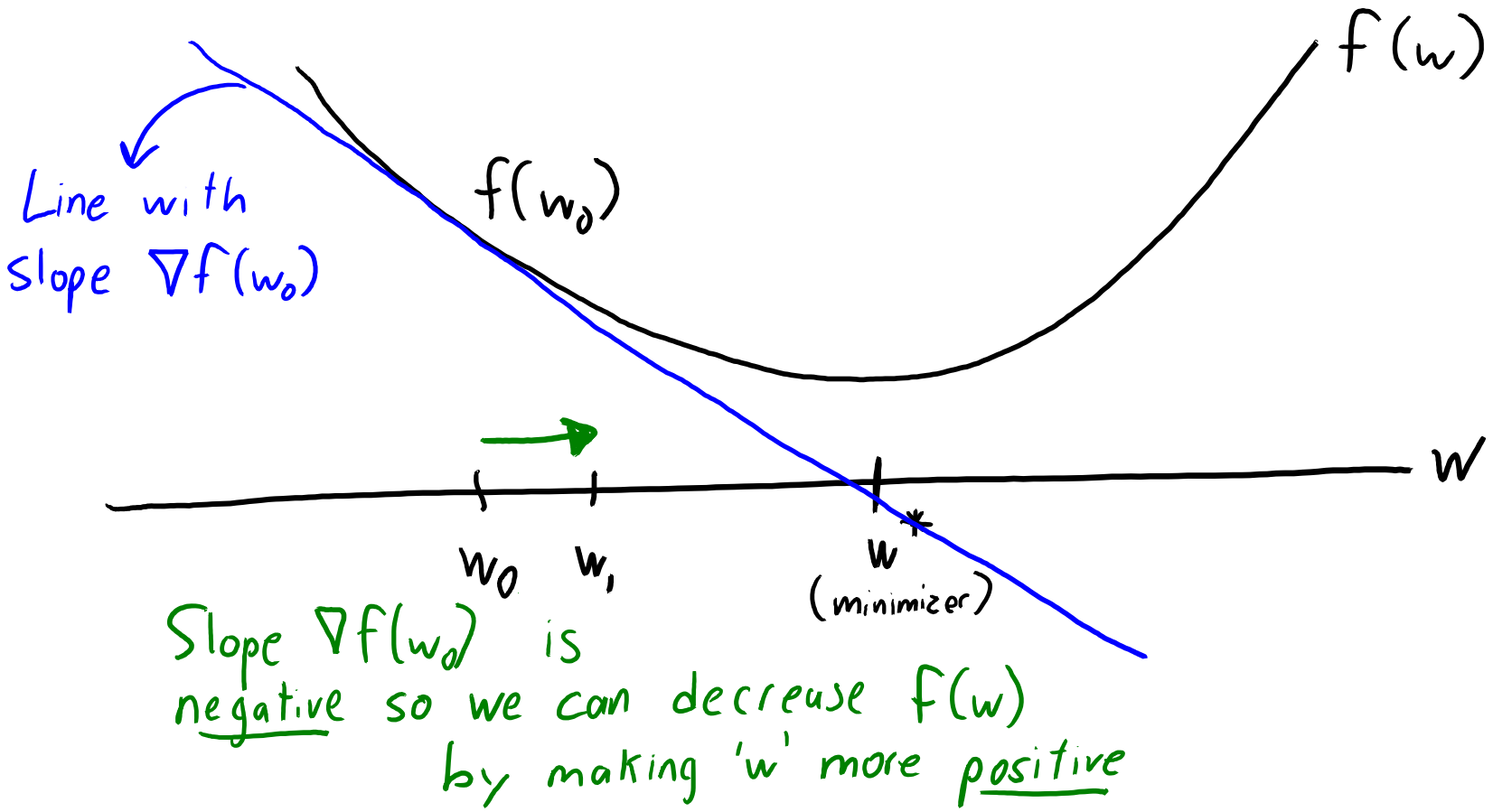

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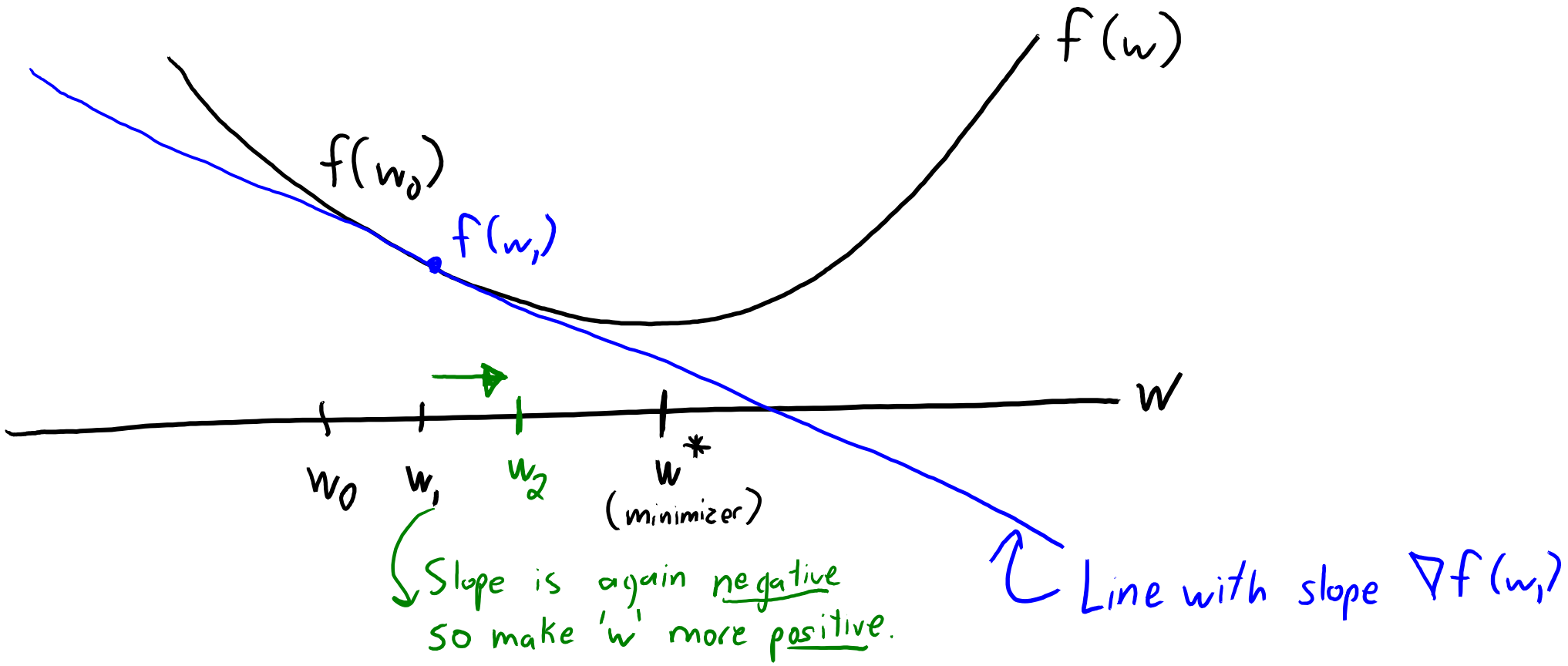

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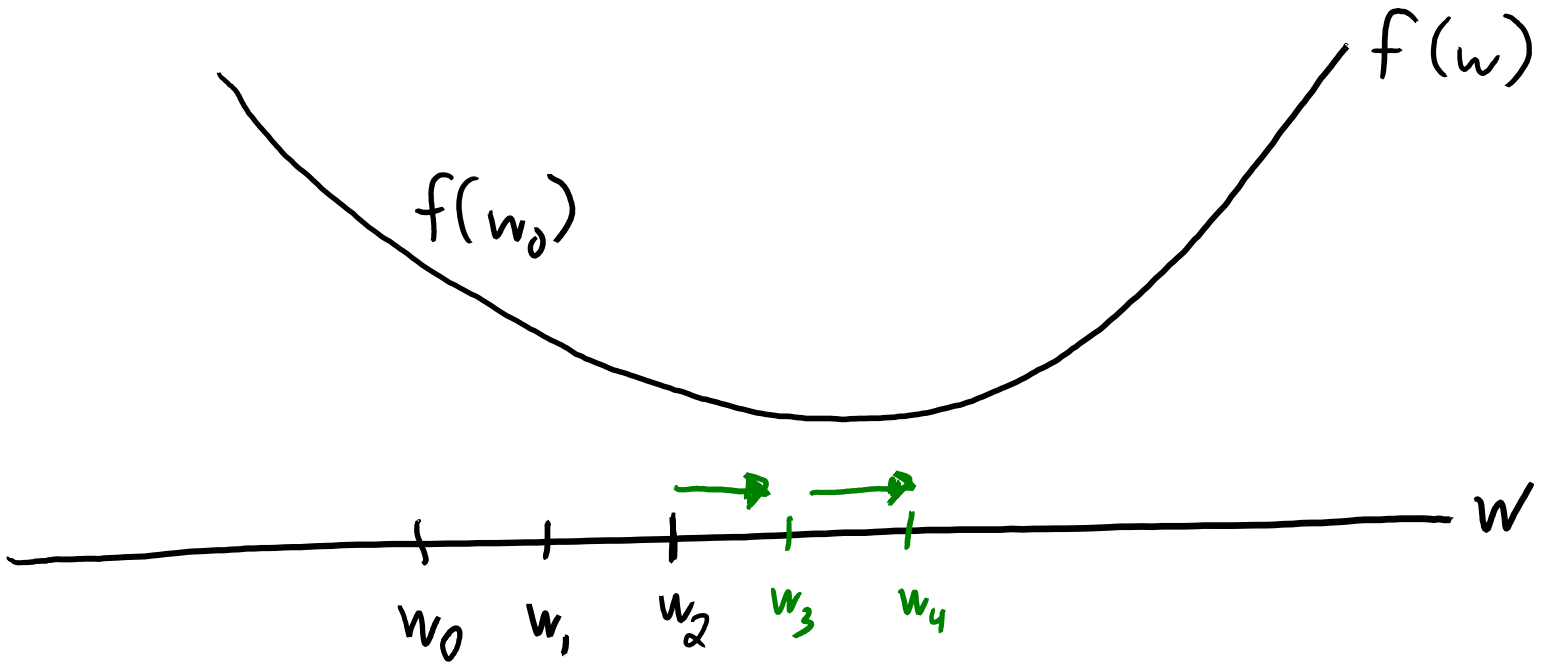

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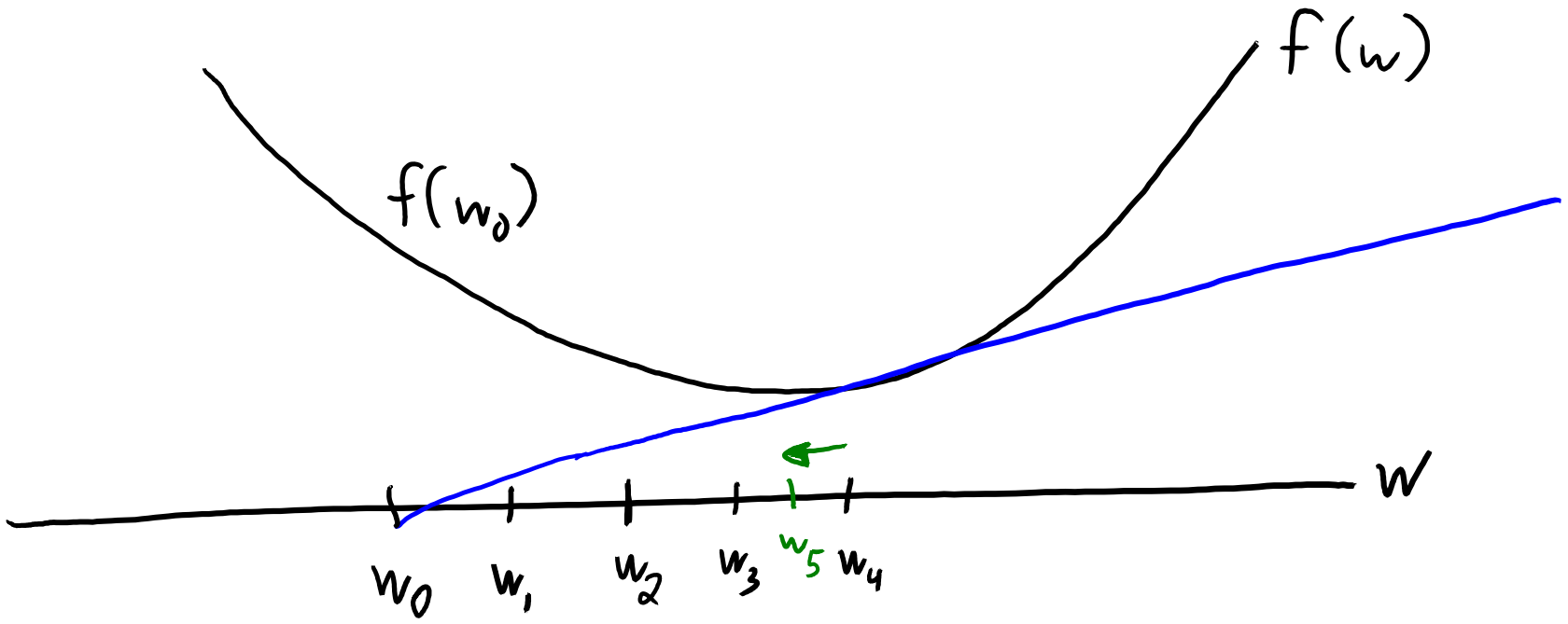
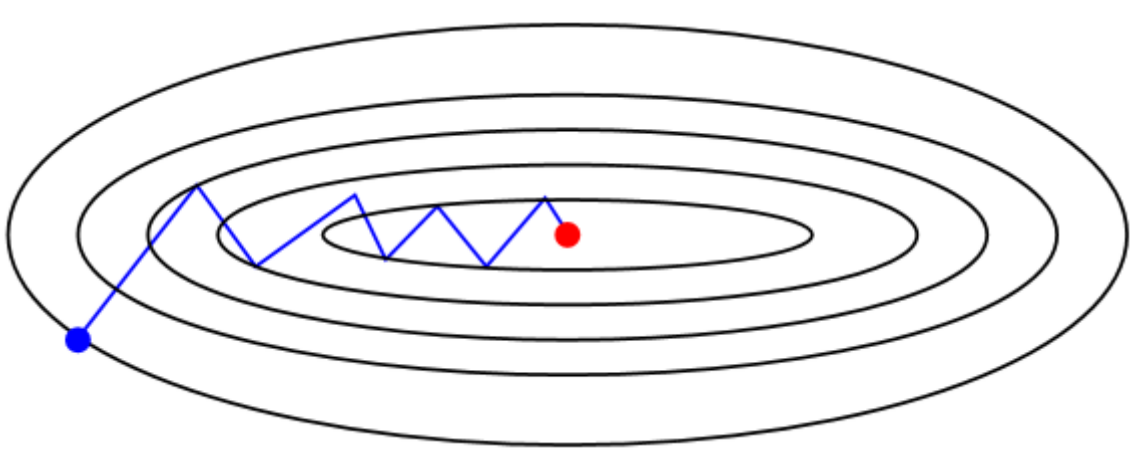
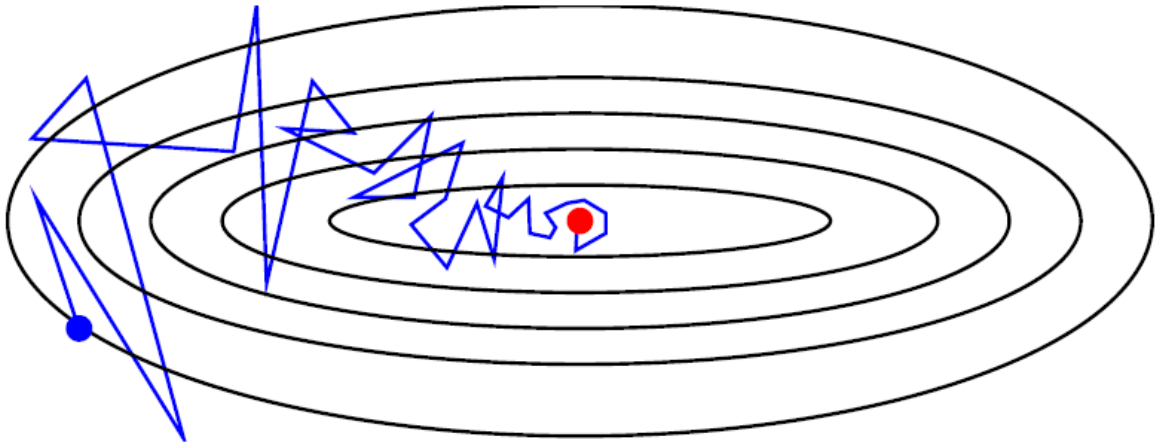


DGD and SGD in 2 Dimensions

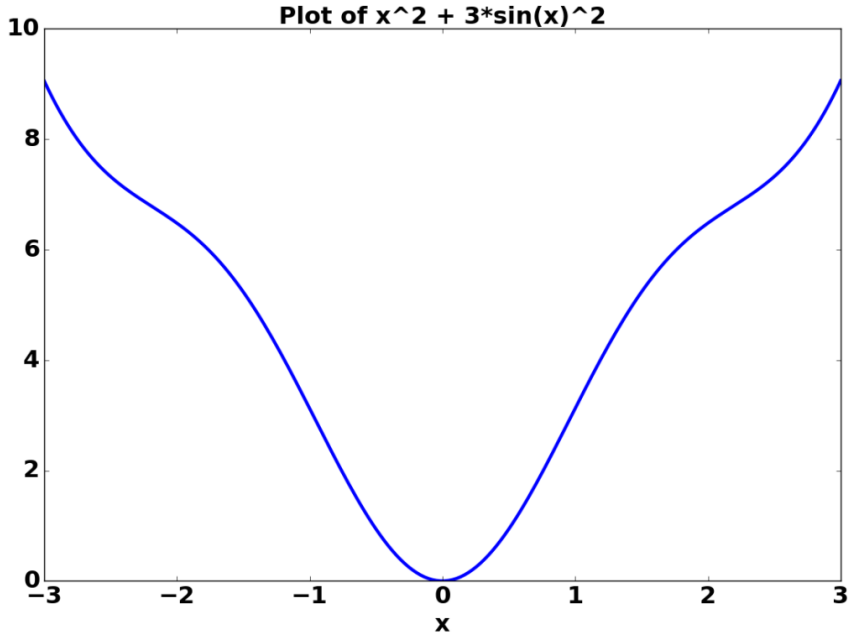




- Deterministic gradient descent (DGD) converges with constant α_k.
- Stochastic gradient descent (SGD) converges with decreasing α_k.
- Both methods are local optimization methods:
  - May not find the global mimimum.
  - But with appropriate step sizes, we have that $\nabla f(w_k)$ converges to 0.

Polyak-Lojasiewicz Inequality and Invexity

- For some functions, we can show that DGD/SGD find a global minimum.



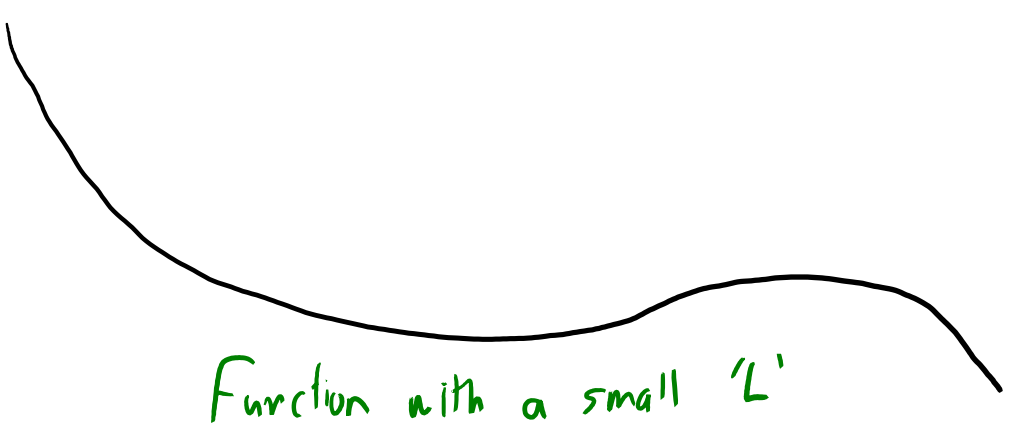
- Recent works argue that some deep learning problems satisfy PL inequality.
  - Polyak-Lojasiewicz inequality.
    - "Gradient increases at least quadratically as we increase f(w) above global minima".
  - PL condition implies invexity.
    - Invexity is a generalization of convexity, where $\nabla f(w_k) = 0$ implies that w_k is a global min.

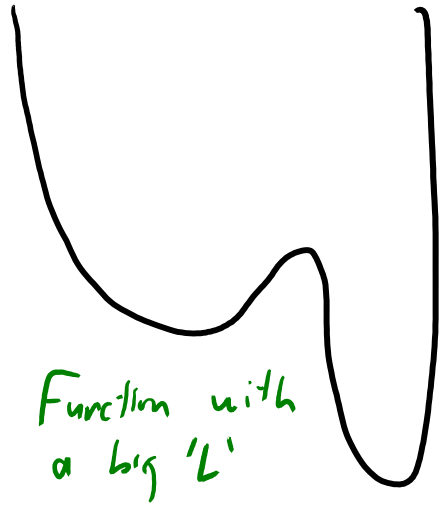
Question 1: How do I set the step size?

- For gradient descent, there is a trade-off between:

α_k "step size" vs. $\frac{2}{L}$ "Lipschitz constant of gradient"

- The number 'L' is how fast the gradient can change:
  - The "Lipschitz constant": $\left|\left|\nabla f(w) - \nabla f(v)\right|\right| \leq L||w - v||$





  - Need smaller steps for bigger 'L'.

Question 1: How do I set the step size?

- For gradient descent, there is a trade-off between:

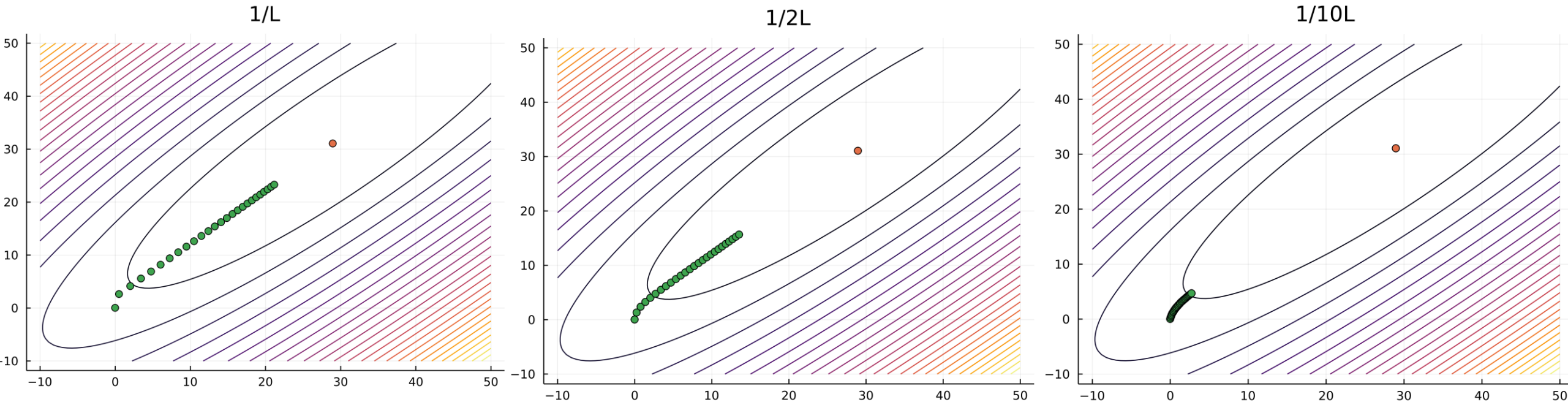
α_k vs. $\frac{2}{L}$

"step size" "Lipschitz constant of gradient"

- If $\alpha_k < 2/L$, DGD is guaranteed to decrease the function 'f'.
- If α_k is much smaller than 2/L, DGD will converge more slowly.
  - Step size is too small.
- If α_k is bigger than 2/L, you might increase the function.
  - Step could be too big and "overshoot" region where function decreases.
  - But you might get lucky and decrease the function a lot.
    - In practice, people use clever step sizes or line searches to make DGD work well.

Comparison of Fixed Step Sizes for DGD

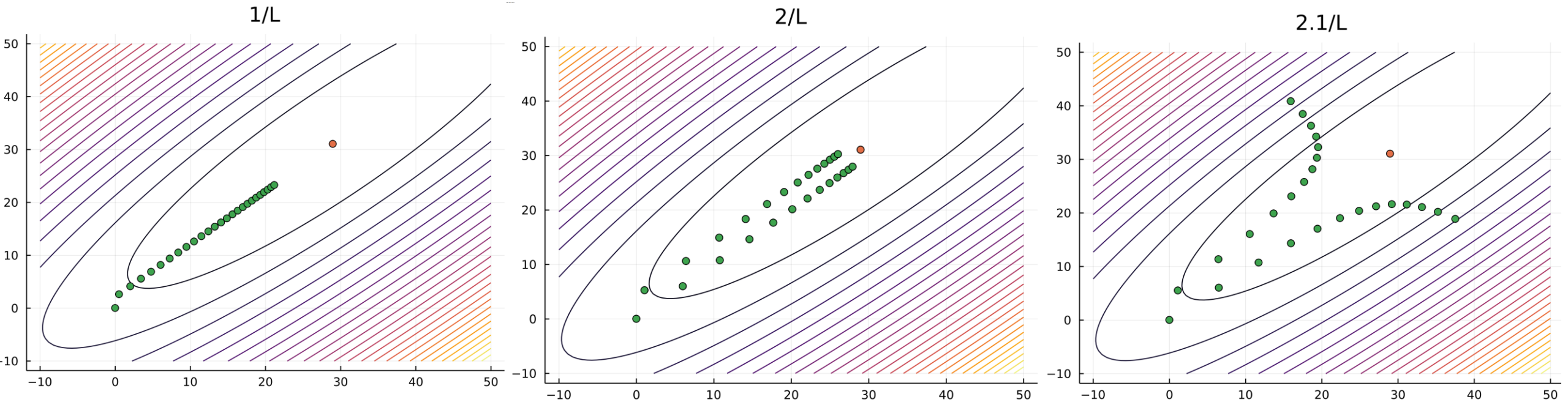
- 25 steps of deterministic gradient descent with different α_k.



- Progress is very slow if α_k is too small.

Comparison of Fixed Step Sizes for DGD

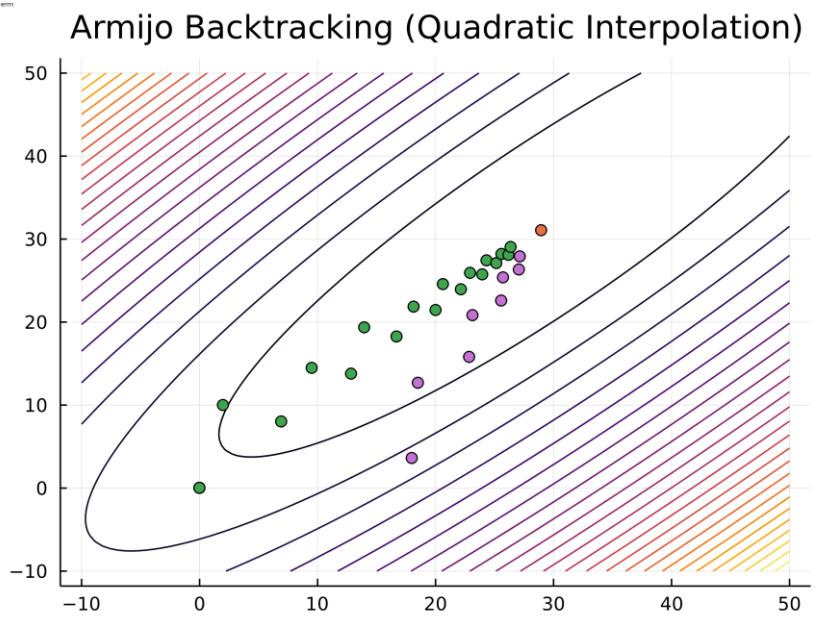
- Increasing the step size:

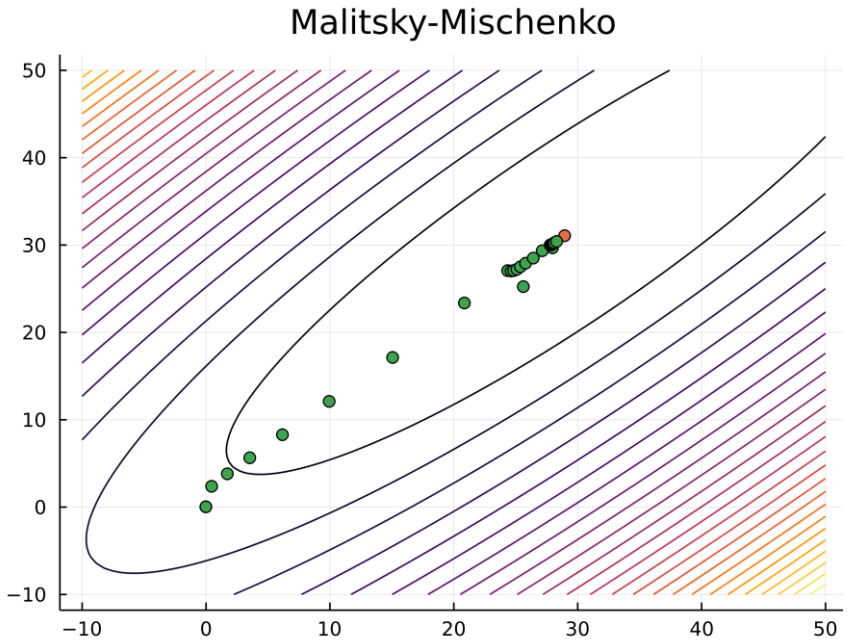


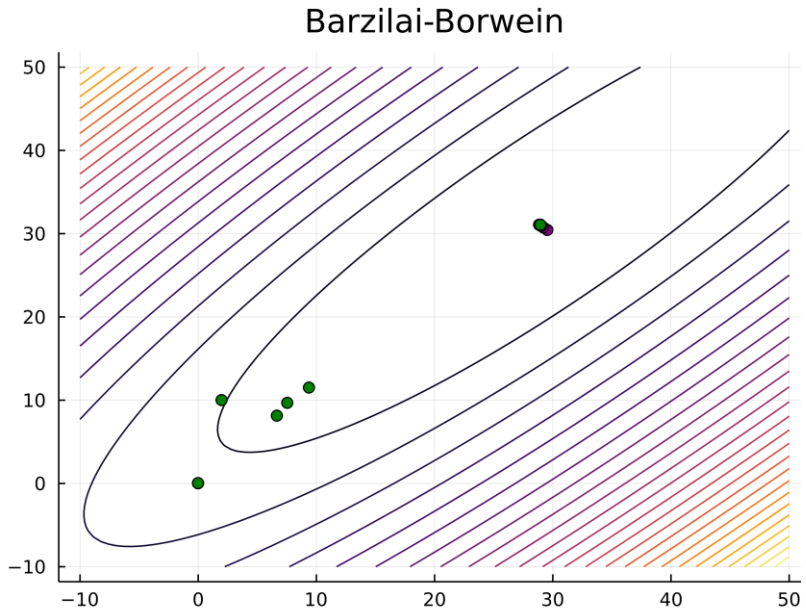
- Progress can be faster if $\alpha_k \geq 2/L$ or it may may increase function.

Comparison of Adaptive Step Sizes for DGD

- For DGD you can also use clever step sizes or line-searches.







- Better than fixed steps in practice, do not work for SGD in general.

Question 1b: How do I set the SGD step size?

- For stochastic gradient descent, there is a second trade-off:

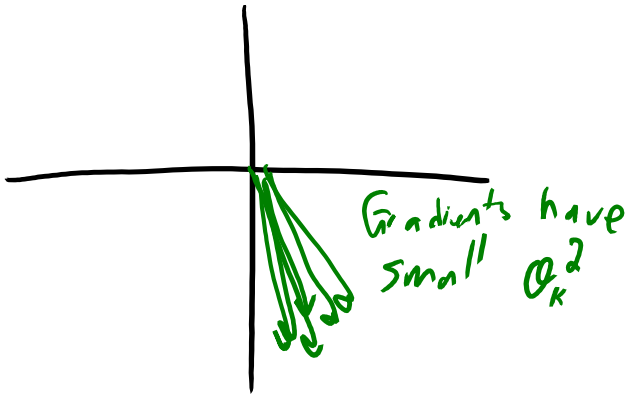
$\|\nabla f(w_k)\|^2$ vs. $\alpha_k \sigma_k^2$

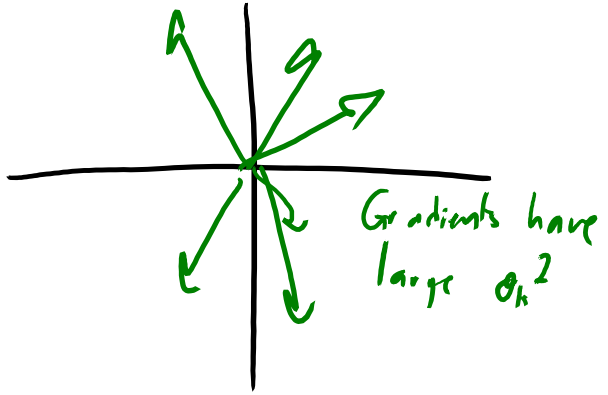
"size of gradient of overall function"

step size

"variation in the stochastic gradients"

- The number σ_k^2 measures the variation in the gradients.
  - We have $\sigma_k^2 = \frac{1}{n}\sum_{i=1}^{n} \|\nabla f_i(w^k) - \nabla f(w^k)\|^2$.





  - Need smaller steps for bigger σ_k^2 (but also depends on $\|\nabla f(w_k)\|$).

Question 1b: How do I set the SGD step size?

- For stochastic gradient descent, there is a second trade-off:

$\|\nabla f(w_k)\|^2$ vs. $\alpha_k \sigma_k^2$

"size of gradient of overall function"

α_k: step size

σ_k^2: "variation in the stochastic gradients"

- If $\left\|\|\nabla f(w_k)\|\right\|^2 \gg \alpha_k \sigma_k^2$, SGD is guaranteed to decrease expected 'f'.
  - As long as we still have $\alpha_k < 2/L$.
  - For DGD, we do not need to worry about this trade-off because $\sigma_k = 0$.
- If $\alpha_k \sigma_k^2 \gg \left\|\|\nabla f(w_k)\|\right\|^2$, noise in SGD makes us increase expected 'f'.
  - Step size if too big, causing the noise to interfere with progress.
  - Need to decrease step size to re-gain progress, but this slows down convergence.

Question 1b: How do I set the SGD step size?

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$\|\nabla f(w_k)\|^2$ vs. $\alpha_k \sigma_k^2$

"size of gradient of overall function"

step size

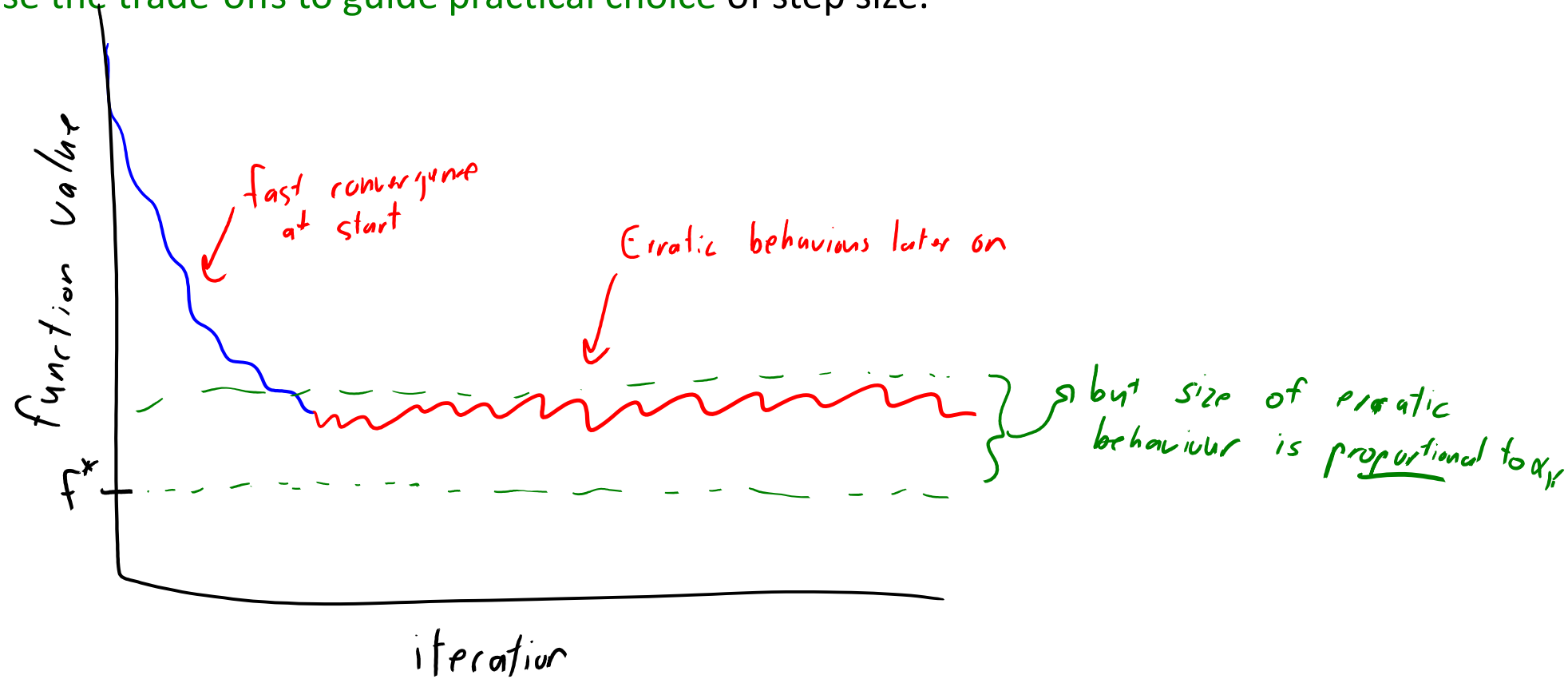
"variation in the stochastic gradients"

- Optimization: we want $\nabla f(w_k)$ to converge to 0 as 'k' grows.
  - So we need to use decreasing step sizes to guarantee continued progress.
    - But as we decrease the step size SGD will converge slower.

- Machine learning: we only need $\nabla f(w_k)$ to close to 0.
  - We expect test error to similar for all w_k "close enough" to stationary point.
    - If you measure the test error to 2 decimal places, may not need 10 decimal places of accuracy.
  - For any "closeness", we could use a small-enough constant step size $\alpha_k = \alpha$.
    - Guarantees progress until $\nabla f(w_k)$ is "close enough" to zero.
    - But in areas where gradient is small, SGD can behave erratically.

Question 1b: How do I set the SGD step size?

- In practice, SGD algorithm does not have access to $\nabla f(w_k)$ or σ_k.
  - But we can use the trade-offs to guide practical choice of step size.



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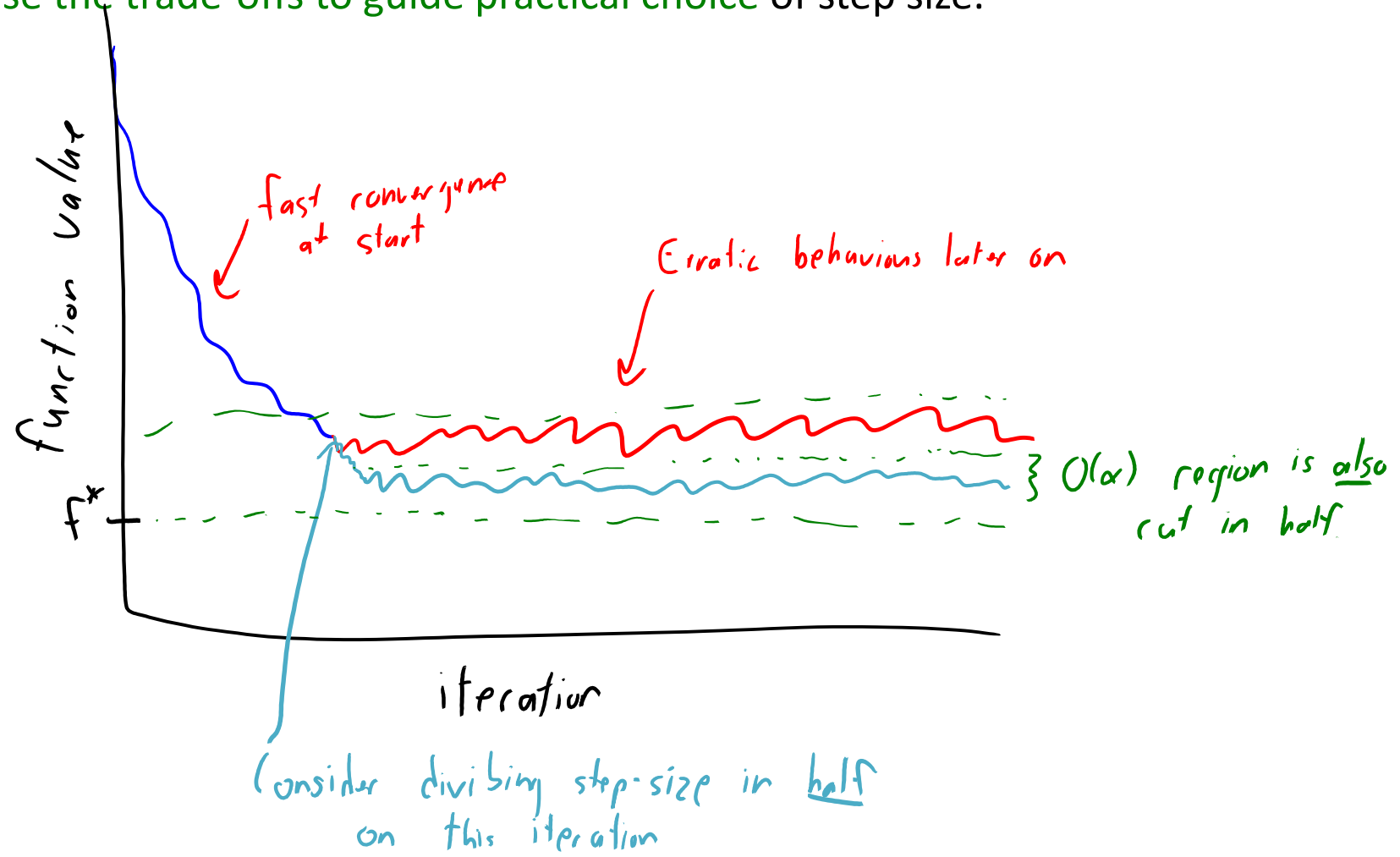


Question 2: How do I pick the mini-batch size?

- Instead 1 random example, we often use a mini-batch in SGD:

$$w_{k+1} = w_k - \alpha_k \left(\frac{1}{|B_k|} \sum_{i \in B_k} \nabla f_i(w_k) \right)$$

average gradient on a mini-batch of examples

  - We can often compute gradient of many examples in parallel.
  - The mini-batch gives a better approximation of true gradient $\nabla f(w_k)$.
- With random mini-batches, second part of trade-off changes to:

$$\|\nabla f(w_k)\|^2 \quad \text{vs.} \quad \frac{\alpha_k \sigma_k^2}{|B_k|}$$

size of mini-batch

  - "With a mini-batch size of 100, effect of noise is divided by 100."
  - "With a mini-batch size of 100, you can use a step size that 100-times larger."
    - As long as the step size is still less than 2/L.

Question 2b: How do I grow the mini-batch size?

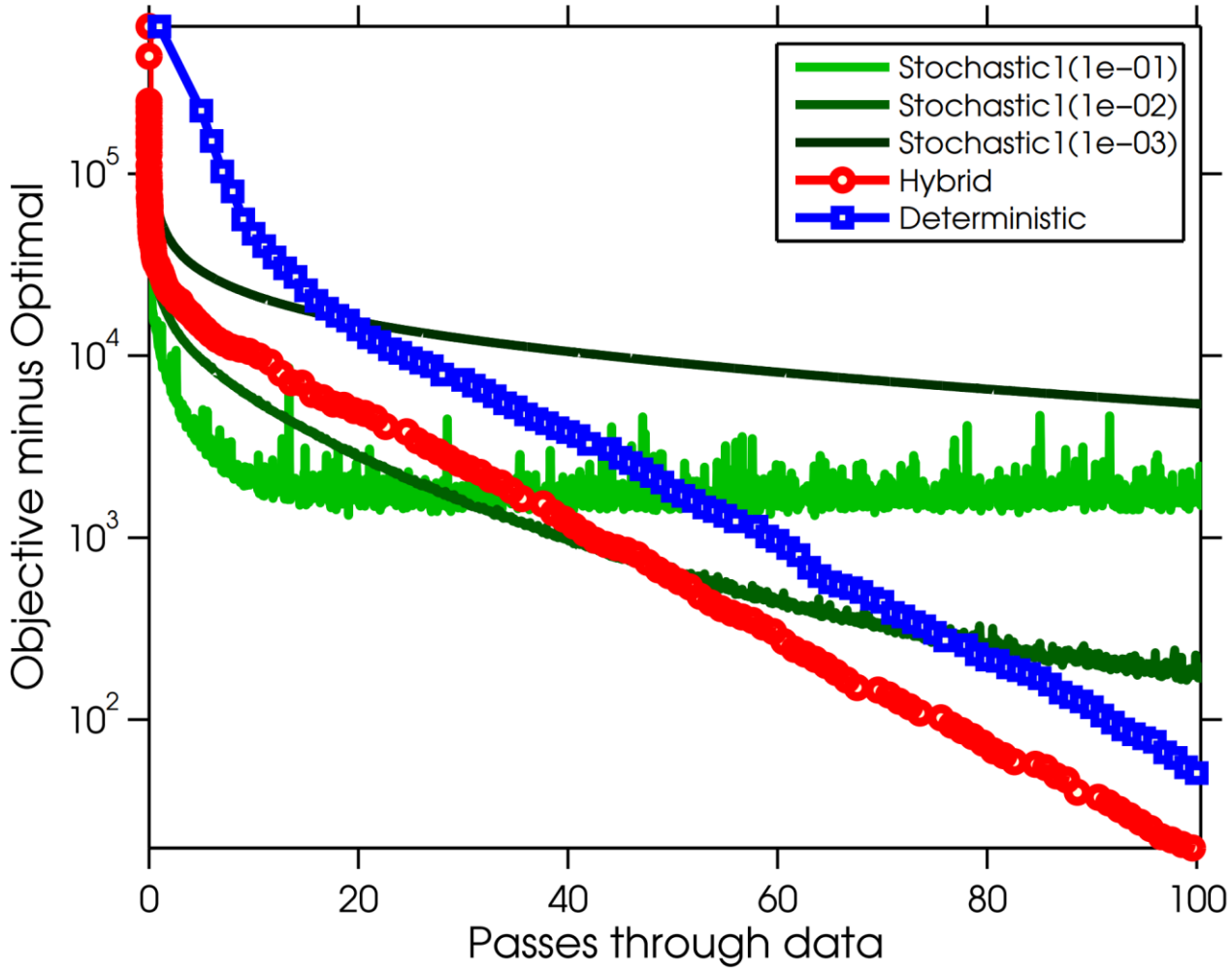
- If $\left|\left|\nabla f(w_k)\right|\right|^2 \gg \alpha_k \sigma_k^2 / |\mathrm{B_k}|$, mini-batch SGD guarantees progress.
  - Again, you can decrease α_k to continue progress as $\nabla f(w_k)$ goes to 0.
  - Or, you can increase the batch size $|B_k|$ as $\nabla f(w_k)$ goes to 0 ("batching").
    - Growing batch sizes gives convergence with a constant step size.
- The situation is better if you have a finite data set.
  - If you sample mini-batch without replacement from 'n' examples:

$||\nabla f(w_k)||^2$ vs. $\frac{\alpha_k \sigma_k^2}{|B_k|} \frac{(n - |B_k|)}{n}$ → "finite sample correction"

  - Drives the effect of σ to 0 as $|B_k|$ approaches 'n' (instead of ∞).
- Growing batches allow using clever step sizes and line-searches.

Comparison of Deterministic, Stochastic, and Hybrid

- Comparing DGD to SGD and a growing batch (“hybrid”) method:



Question 3: Should I use variance reduction?

- SGD with a growing batch size ("batching"):
  - Use an estimate of $\nabla f(w_k)$ where σ_k converges to 0 as w_k goes to w_*.
  - But batching may lose low iteration cost of SGD.

- Variance-reduced stochastic gradient methods (like SAG and SVRG):
  - Design an estimate of $\nabla f(w_k)$ where σ_k converges to 0 as w_k goes to w_*.
  - But only need 1 random example per iteration.
    - So these methods have the low iteration cost of SGD.

- Variance-reduced methods remove second part of trade-off.
  - This improves convergence speed a lot for under-parameterized models.
  - But variance reduction is not needed for over-parameterized models.

Over-Parameterized Gradient Descent (OGD)

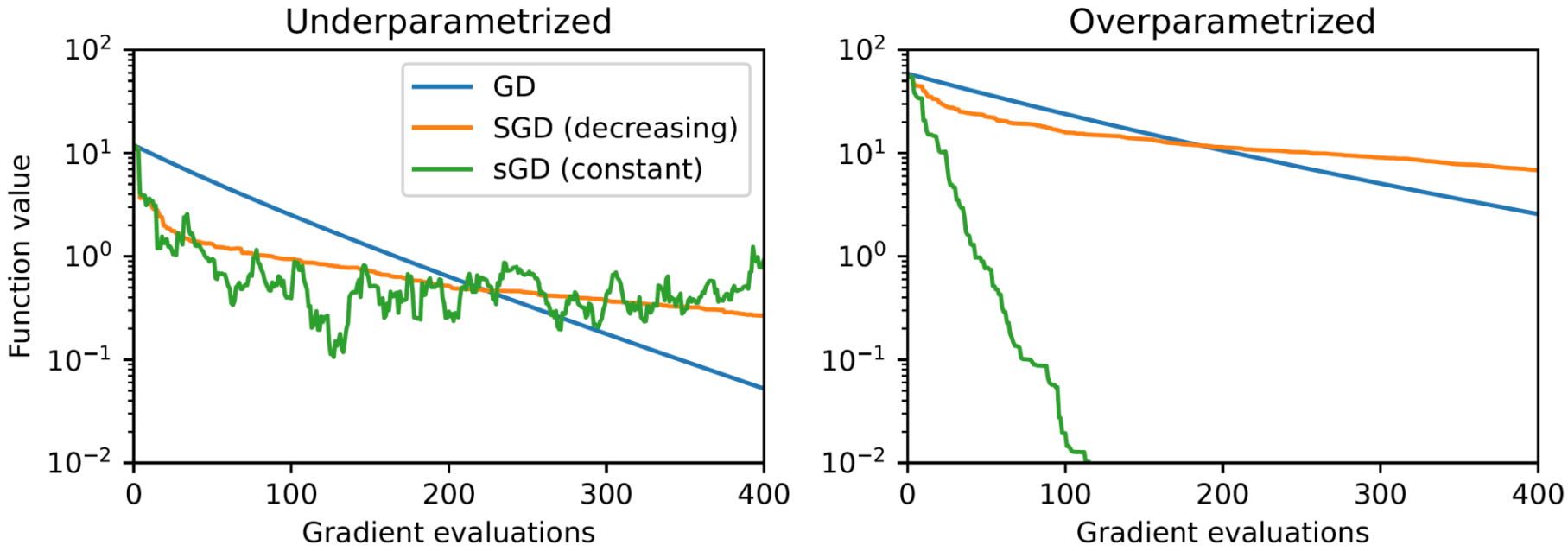
- A model is over-parameterized if it can fit data with training error 0.

- How does this affect optimization?
  - In this setting, when we minimize 'f' we also minimize each 'f_i'.
  - So at a global minimum w_* we have $\nabla f_i(w_*) = 0$ for all 'i'.
  - And this means that $\sigma_*^2 = 0$ (there is no noise at the minimum).
  - So σ_k goes to 0 as $\nabla f(w_k)$ goes to 0.

- I will use term OGD for over-parameterized gradient descent.
  - When we apply SGD with a constant step size to an over-parameterized problem.

Over-Parameterized Gradient Descent (OGD)

- Since σ_k goes to 0, OGD is less affected by the second trade-off.
  - It converges like DGD with the iteration cost of SGD.



  - No need to decrease step sizes or increase batch sizes.
  - Still expect good performance if you are close to being over-parameterized.
    - Will not converge but will get close to solution with large steps, since σ_*^2 will be small.

Question 3: Should I use variance reduction?

- For over-parameterized models:
  - No need for variance reduction, just use OGD.
    - Variance-reduce methods might be slower than SGD with constant step size.

- For under-parameterized models:
  - Variance reduction may lead to faster convergence.

- Example: generative adversarial networks (GANs).
  - GAN loss cannot be driven to zero.
  - So variance-reduced SGD can lead to faster convergence.

Question 1c: How do I adjust the step size?

- Could we somehow adjust the SGD step size as we go?
  - Accounting for both trade-offs and hoping to get "lucky"?

- Lots of methods have been proposed to do this.
  - "Update step size based on some simple statistics".
  - "Do a line-search based on the mini-batch".
  - "Do gradient descent on the step size".
  - Mark being provocative: almost all of these methods are bad.

- Most of these methods have one at least of these problems:
  - Introduce a new hyper-parameter that is just as hard to tune.
  - Do not converge theoretically (can catastrophically fail).
  - Converges theoretically but works badly in practice.
  - Need to assume that σ_k goes to 0.

Question 1c: How do I adjust the step size?

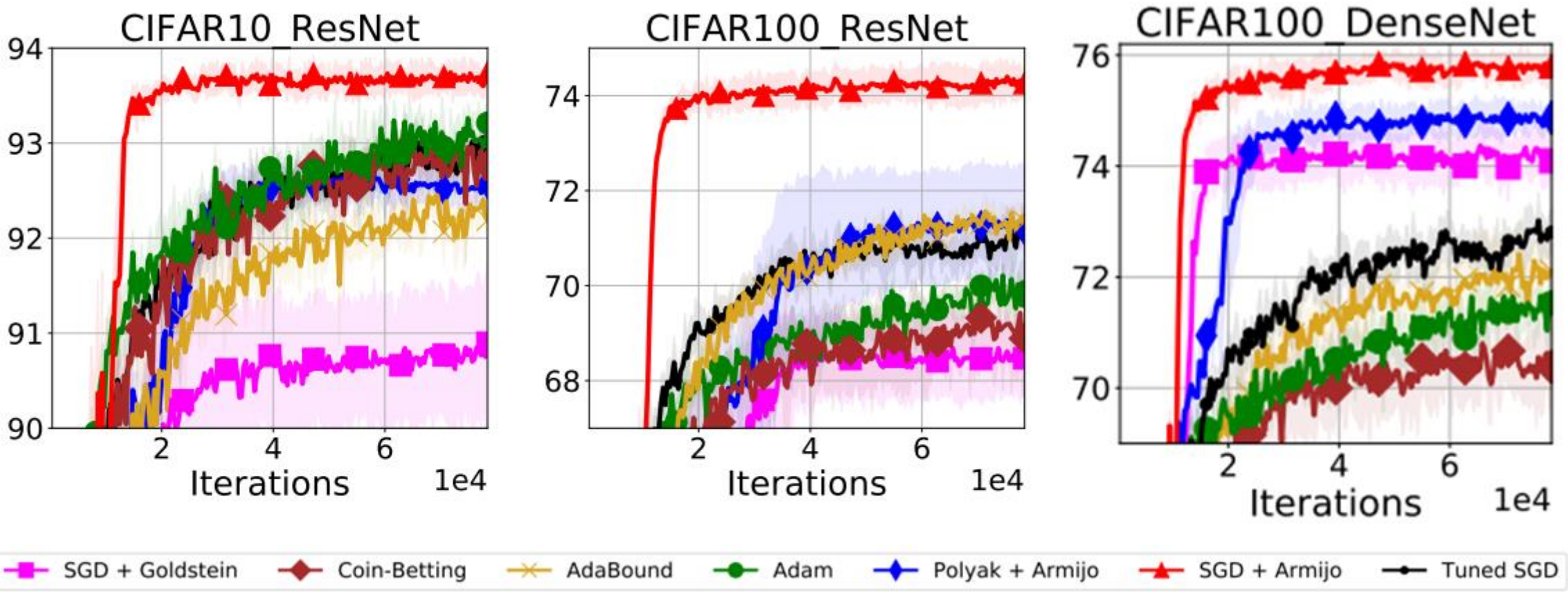
- For under-parameterized problems with fixed batch sizes:
  - I have not had good luck getting anything working well across problems.
    - And I have tried a lot of things over the years.
  - My students say that the recent "coin betting" method works well.
    - And is justified theoretically.

- For over-parameterized problems or batching (where σ_k goes to 0):
  - Can often adapt clever step sizes or line searches designed by DGD.

- Example: for OGD you can use an Armijo backtracking line search.
  - "Decrease step size if it makes less progress than a step size like 1/L would."
  - Theory: "Performs as well or better as best fixed step size" (without knowing 'L').
    - And with careful implementation, cost is less in practice than trying out 2 fixed step sizes.

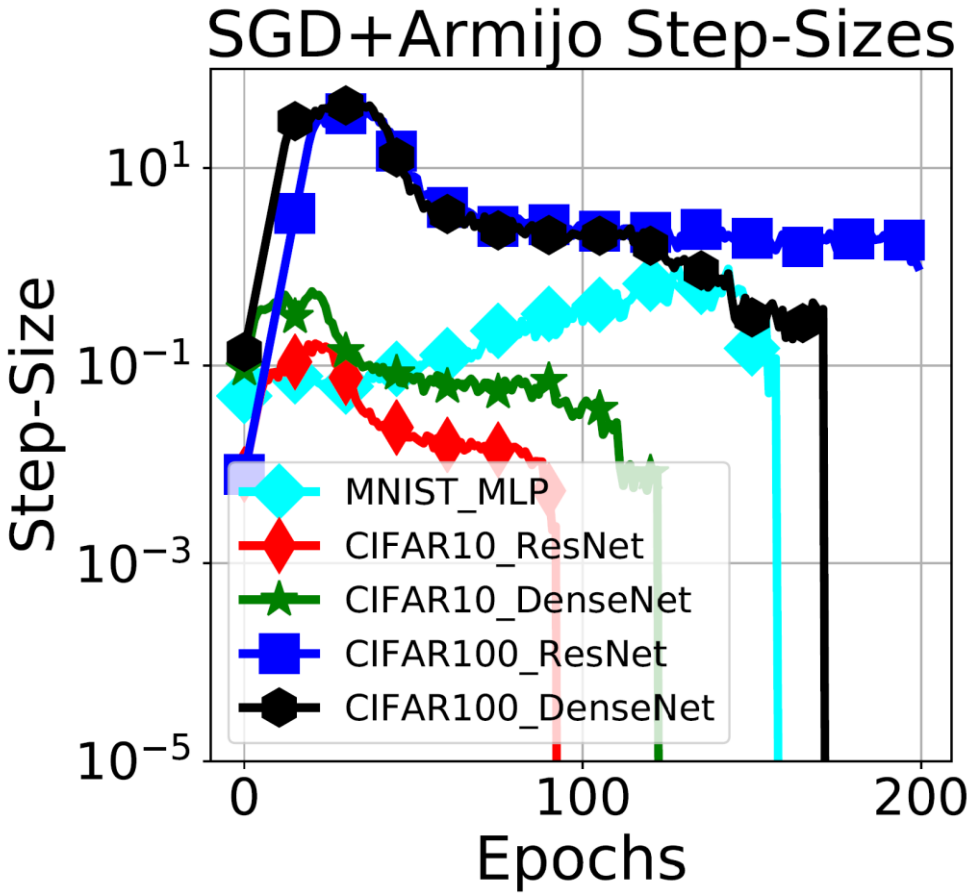
OGD with Armijo Line-Search

- SGD + Armijo outperforms other methods on many benchmarks.



OGD with Armijo Line-Search

- SGD + Armijo outperforms other methods on many benchmarks.
  - Uses different step sizes on different datasets at different times:



Question 4: What about random shuffling?

- How should we choose the random example?
  - Classic SGD theory: must sample i_k uniformly from {1,2,…,n}.
    - Or with importance sampling from a fixed distribution.

- In practice, people often use random shuffling:
  - Compute a random permutation of the training examples.
  - Go through this random permutation in order.
    - Guarantees each example is chosen at least once every ‘n’ iterations.

- Empirical evidence that random shuffling converges faster.
  - Theory is catching up, showing that it likely is always faster.

Question 5: Should I use importance sampling?

- What about sampling i_k from a non-uniform distribution?

- For OGD, importance sampling leads to a faster method:
  - Suppose you know the Lipschitz constant L_i of each training example.
  - OGD converges faster if you bias sampling by the L_i values.
    - "If the gradient of example 'i' can change quickly, sample it more often."
      - For classification problems, the "local" L_i is small if the examples are correctly classified.
    - Normally OGD needs a step size less $2/\max(L_i)$, this allows step sizes less $2/\text{mean}(L_i)$.

- Importance sampling may also help in "low noise" scenarios.
  - But if σ_* is large, we do not expect important sampling to help.

Question 6: Are there faster algorithms?

- We have faster deterministic algorithms than DGD in various setttings:
  - For quadratic functions, we can use the heavy-ball method:

$$w_{k+1} = w_k - \alpha_k \nabla f(w_k) + \beta_k (w_k - w_{k-1})$$

    - Which adds a momentum term to DGD (for some momentum parameter $\beta_k < 1$).
  - For convex functions, we have Nesterov's accelerated gradient method(s):

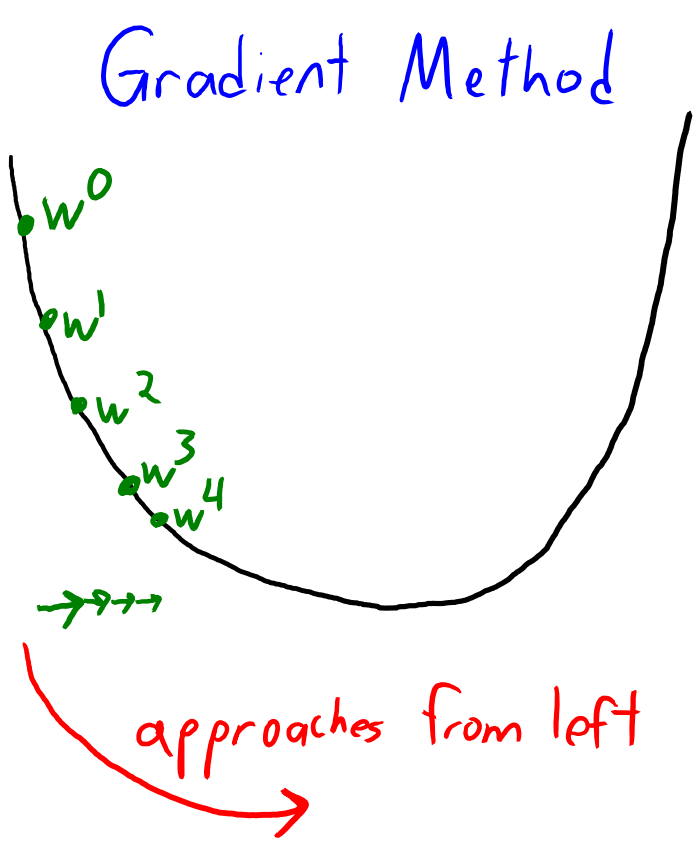
$$w_{k+1} = w_k - \alpha_k \nabla f(w_k) + \beta_k (w_k - w_{k-1}) + \alpha_k \beta_k (\nabla f(w_k) - \nabla f(w_{k-1}))$$

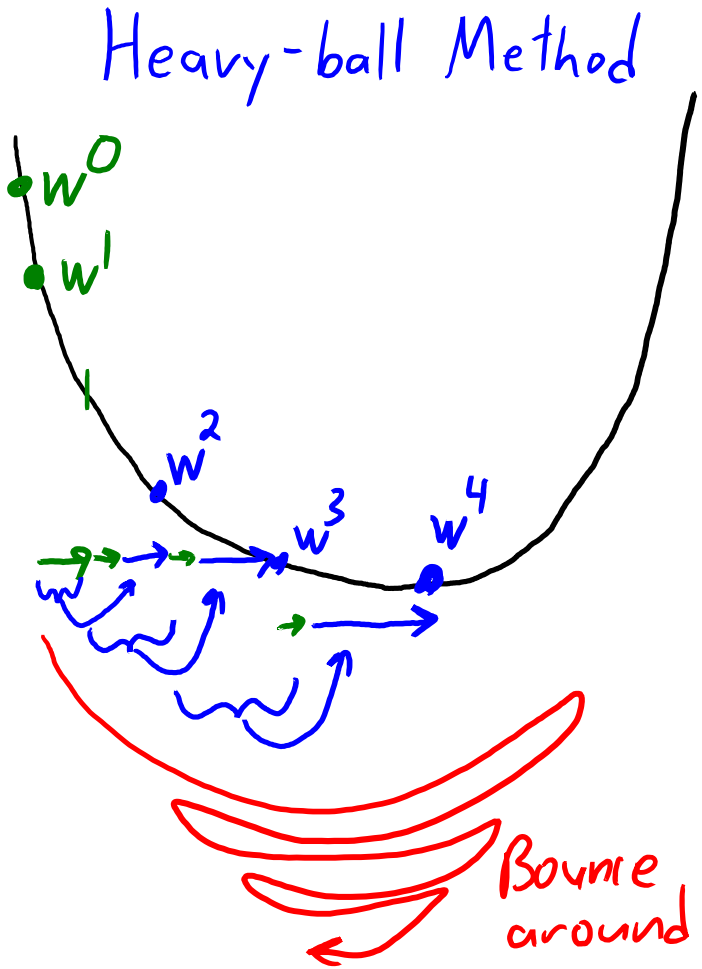
    - Which can add a "gradient difference" to the heavy-ball method.
  - Nearby a strict local minimum, we can use variations on Newton's method:

$$w_{k+1} = w_k - \alpha_k [\nabla^2 f(w_k)]^{-1} \nabla f(w_k)$$

    - Which uses or approximates the second-derivative matrix to converge faster locally.

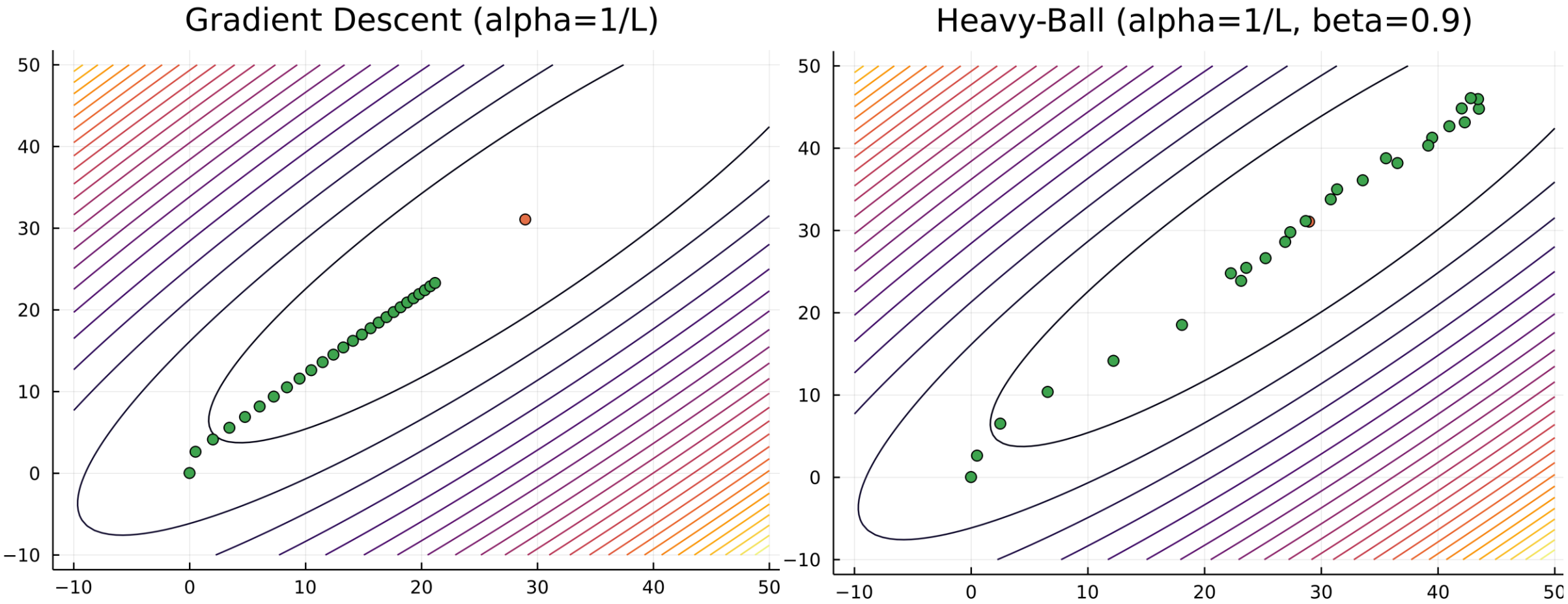
Gradient Descent vs. Heavy-Ball Method





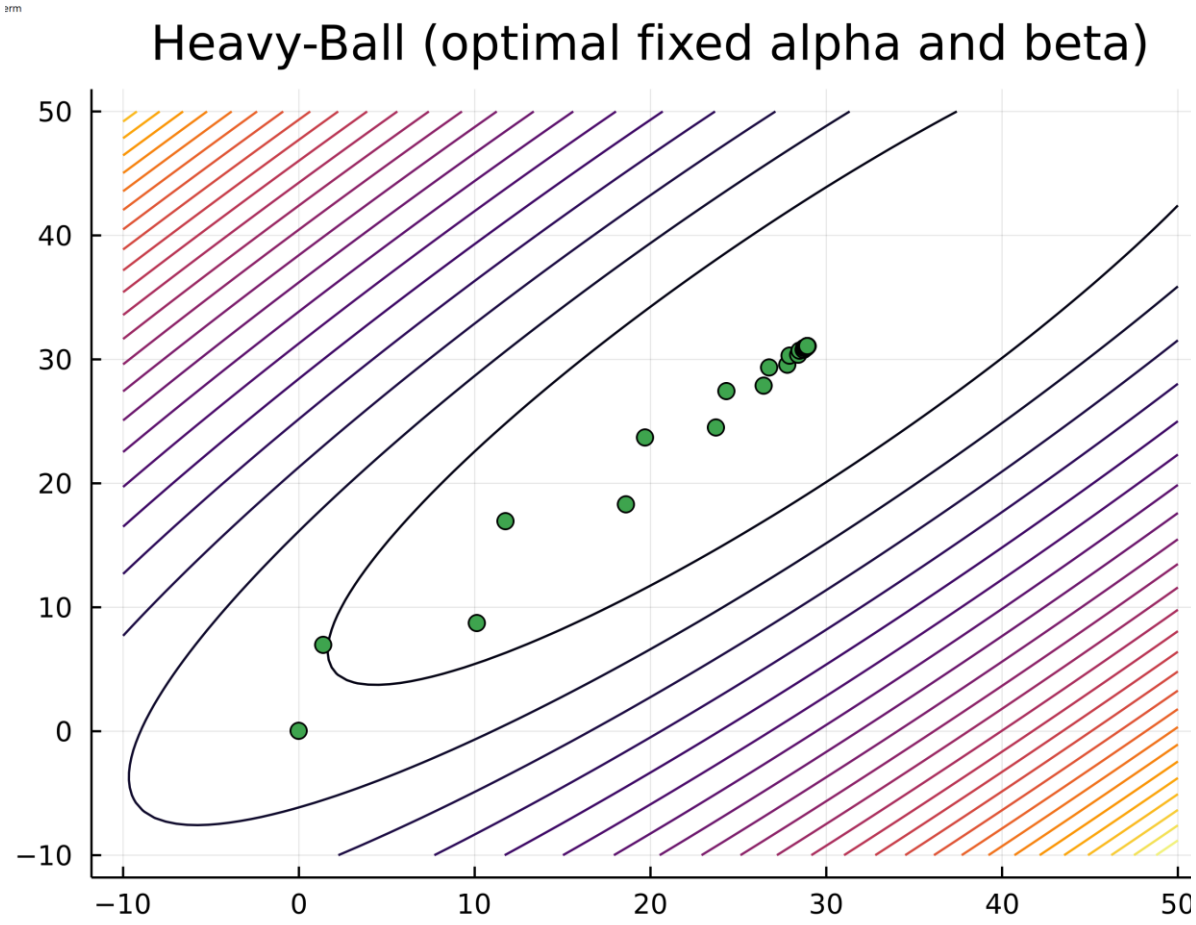
Gradient Descent vs. Heavy-Ball Method

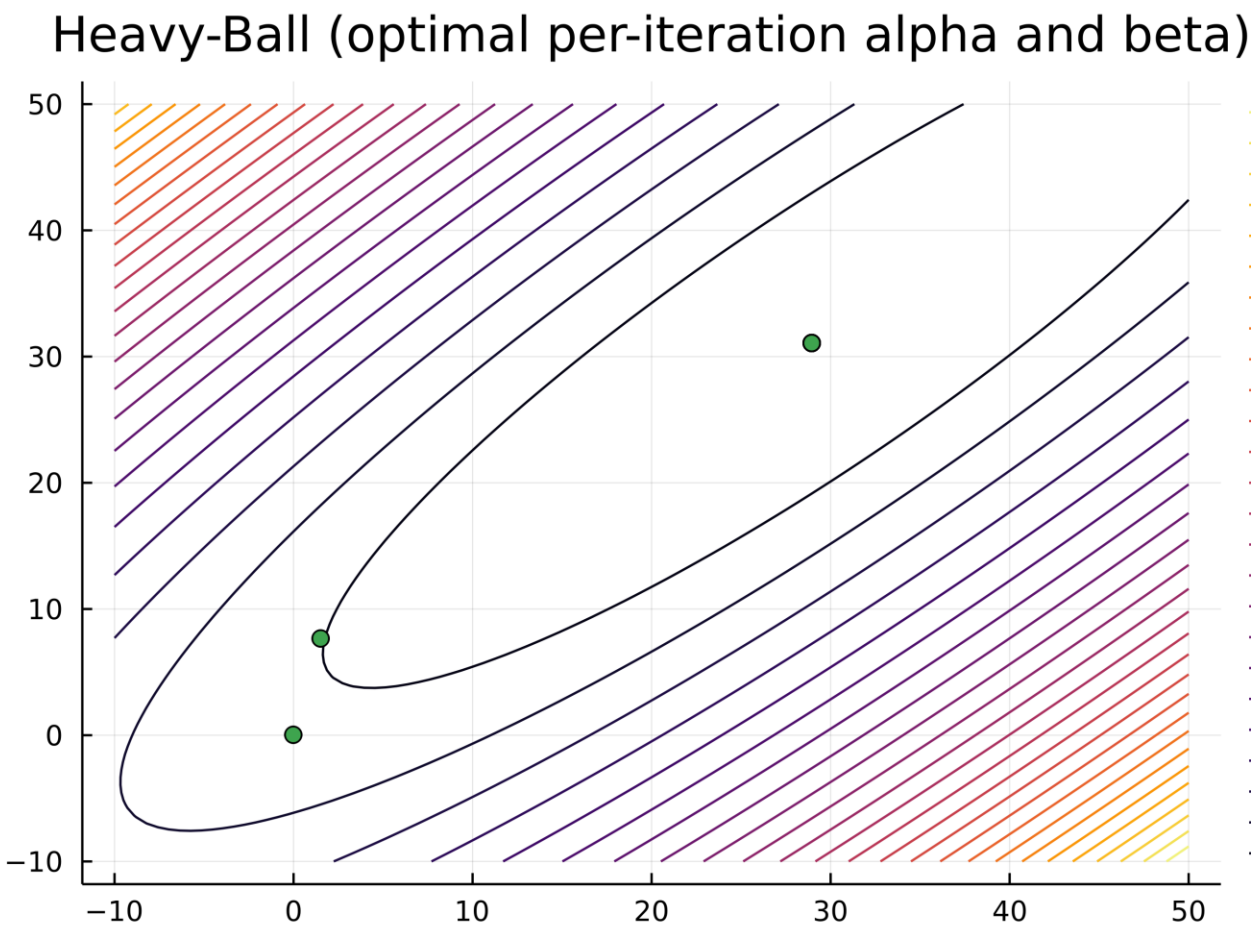
- Adding momentum to DGD with fixed step size and momentum:



Gradient Descent vs. Heavy-Ball Method

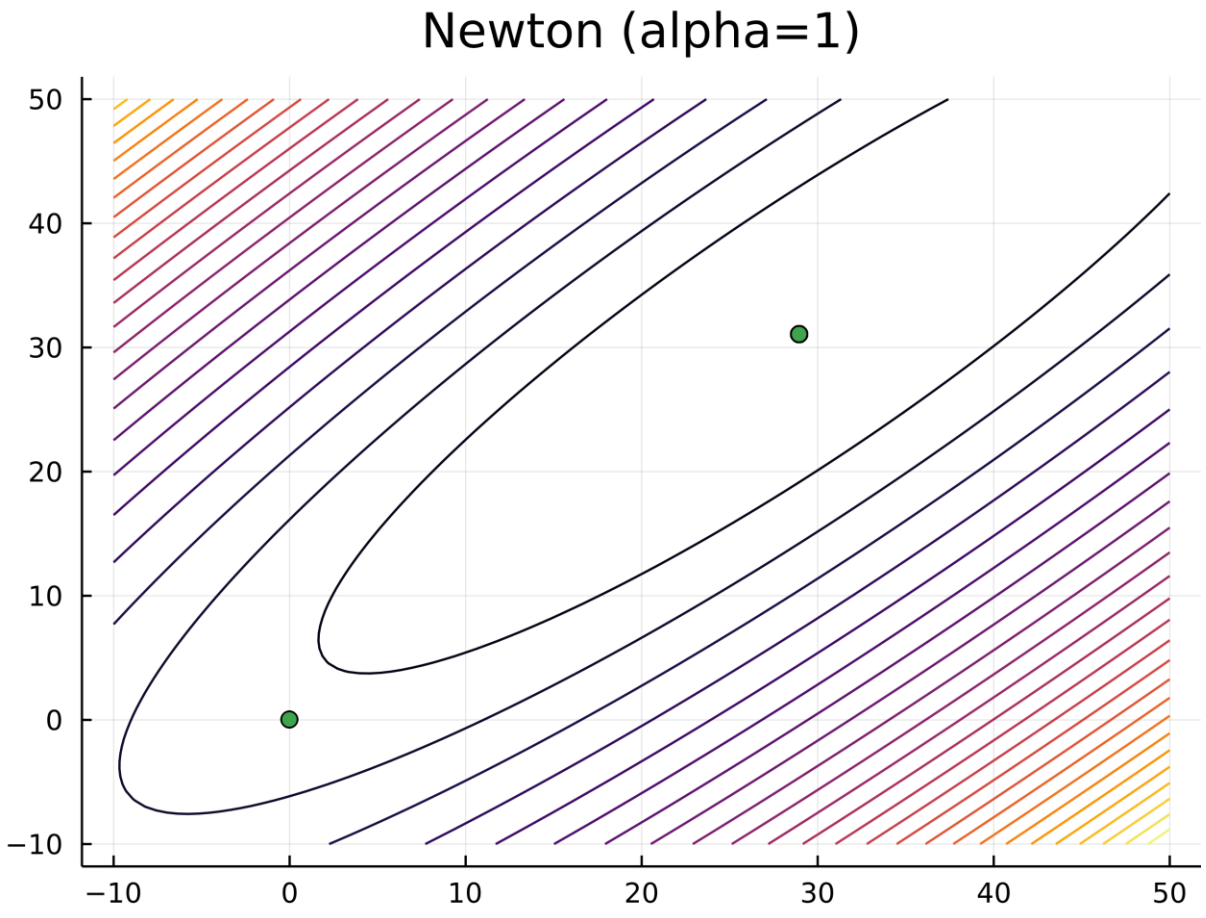
- For deterministic quadratics, exist clever ways to set α_k and β_k.

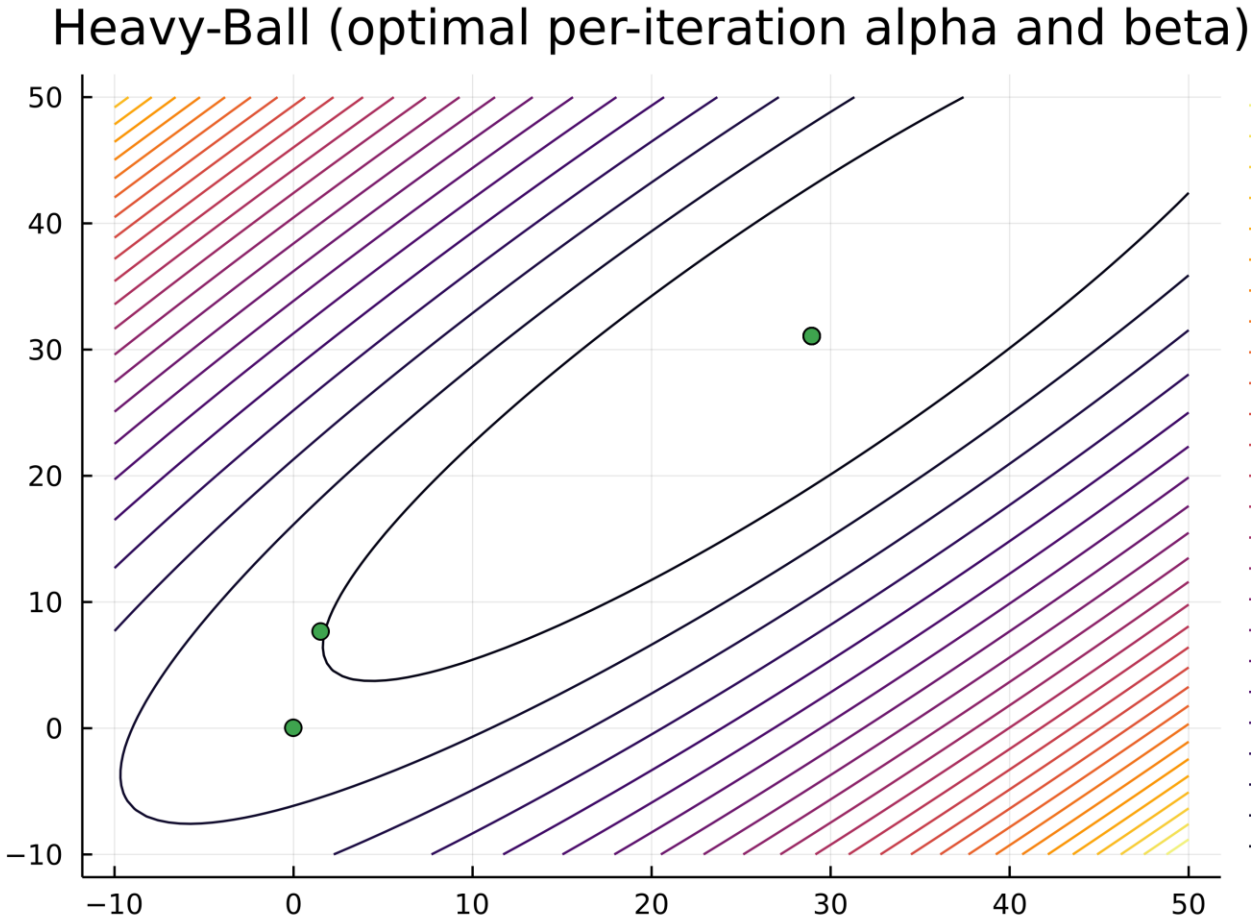




Gradient Descent vs. Heavy-Ball Method

- For deterministic quadratics, Newton converges in 1 step.





Question 6: Are there faster algorithms?

- For over-parameterized or growing batch settings:
  - Ideas like momentum/Nesterov/Newton can make SGD converge faster.

- These faster methods should still work well in low-noise settings.

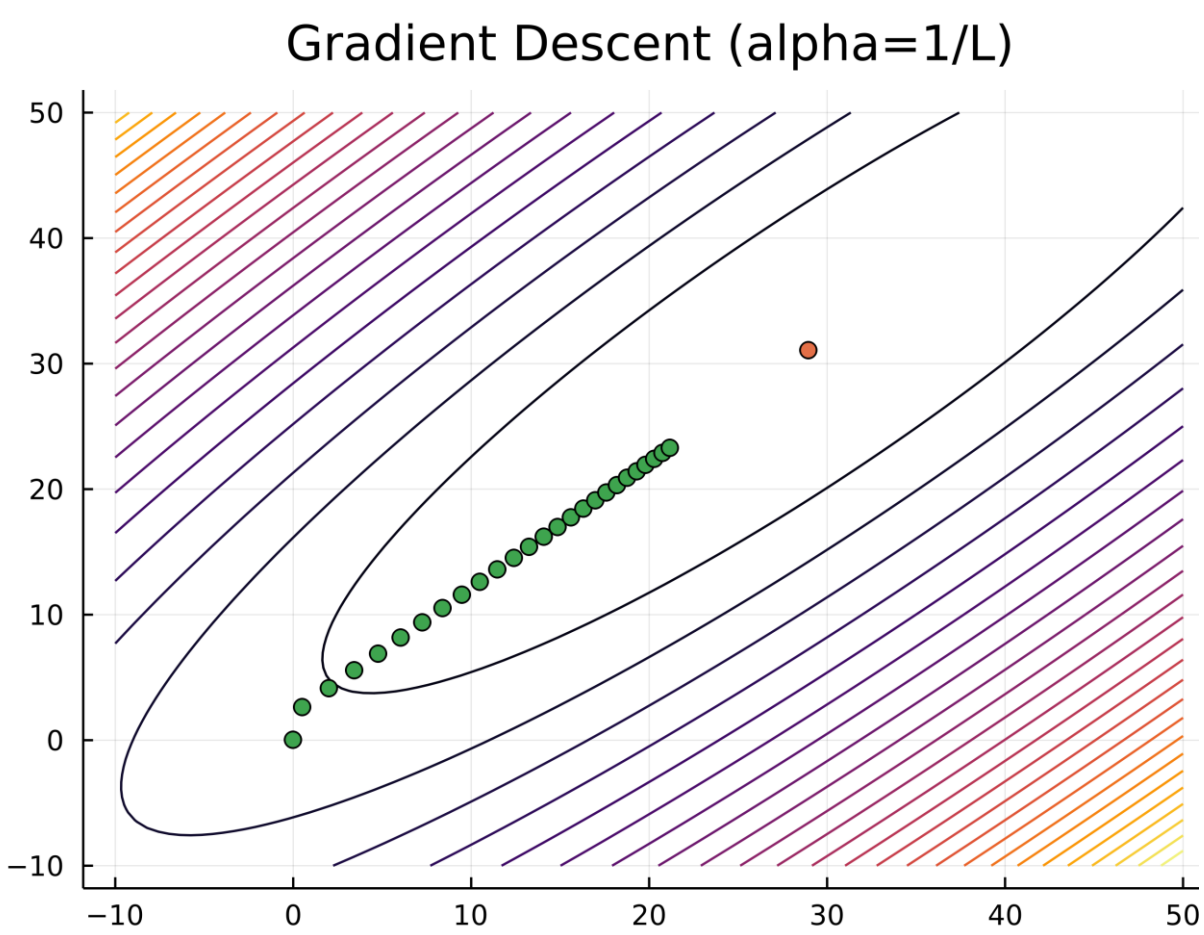
- But these methods do not improve the dependence on σ_k.
  - We do not expect them to converge faster if noise is large.
  - These methods can even amplify the effect of the noise.
    - SGD may need smaller step sizes if you are using momentum.
    - You might need momentum parameter β_k to converge to 0.

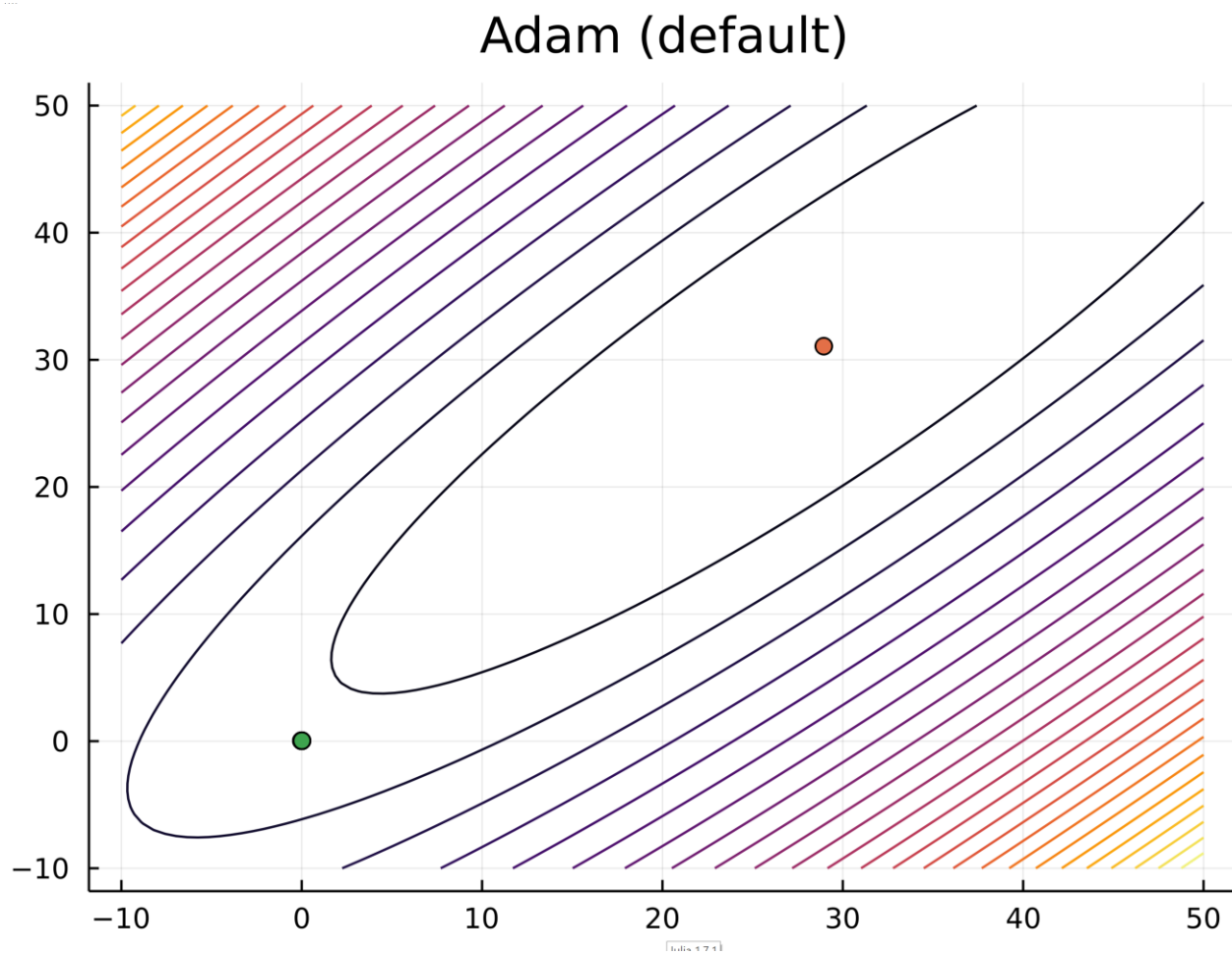
Question 7: Should we just use Adam?

- An extremely popular SGD variant is Adam:
  - Combination of several ideas with good properties in specific settings:
    - AdaGrad which has appealing properties for online learning.
    - Momentum which has appealing properties for deterministic quadratic functions.
    - Step sizes that are constant which has appealing properties for low-noise problems.
- The properties of Adam are not well understood.
  - Analysis in original Adam paper was wrong.
  - There are simple functions where Adam performs terribly.
  - But it is difficult to beat Adam on some architectures like transformers.
  - ??

Gradient Descent vs. Adam

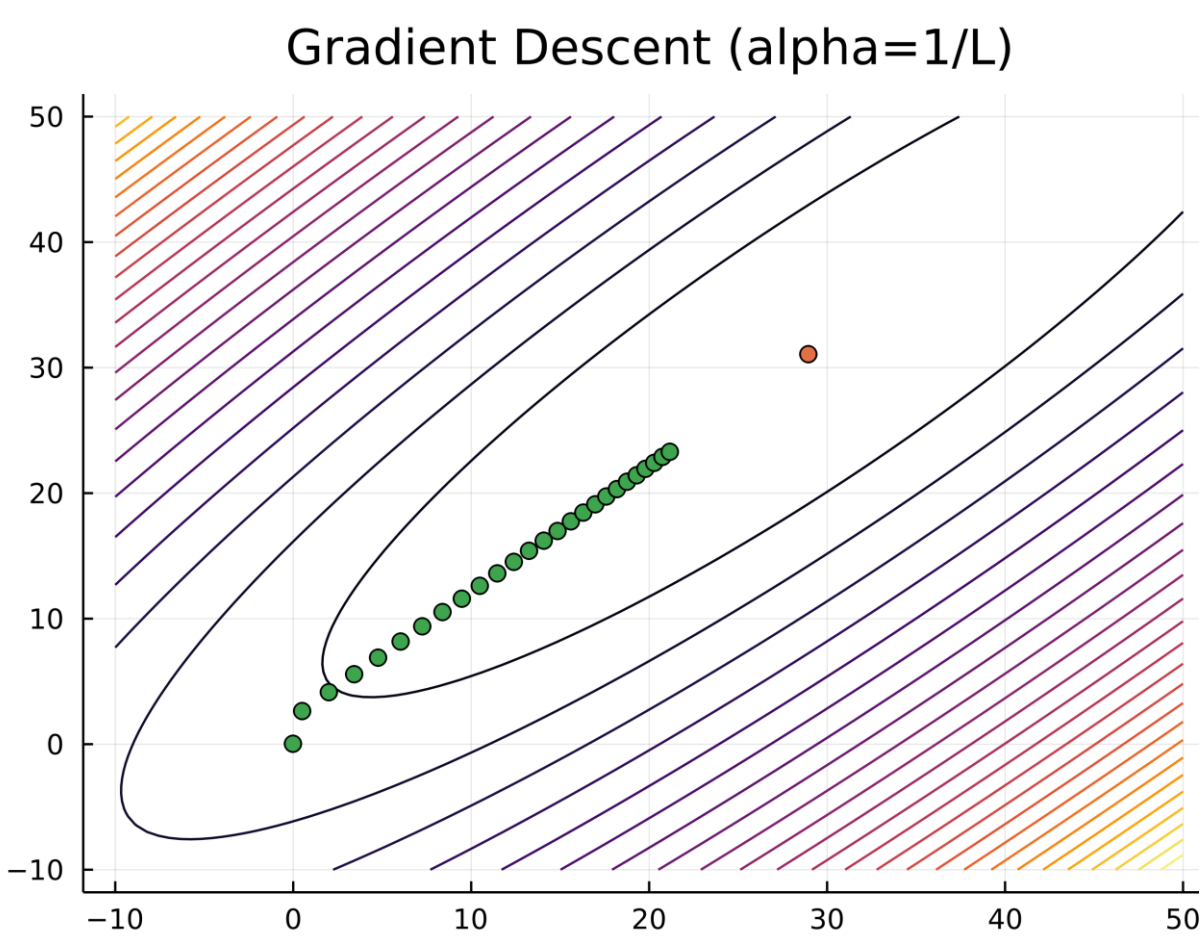
- DGD vs. Adam:

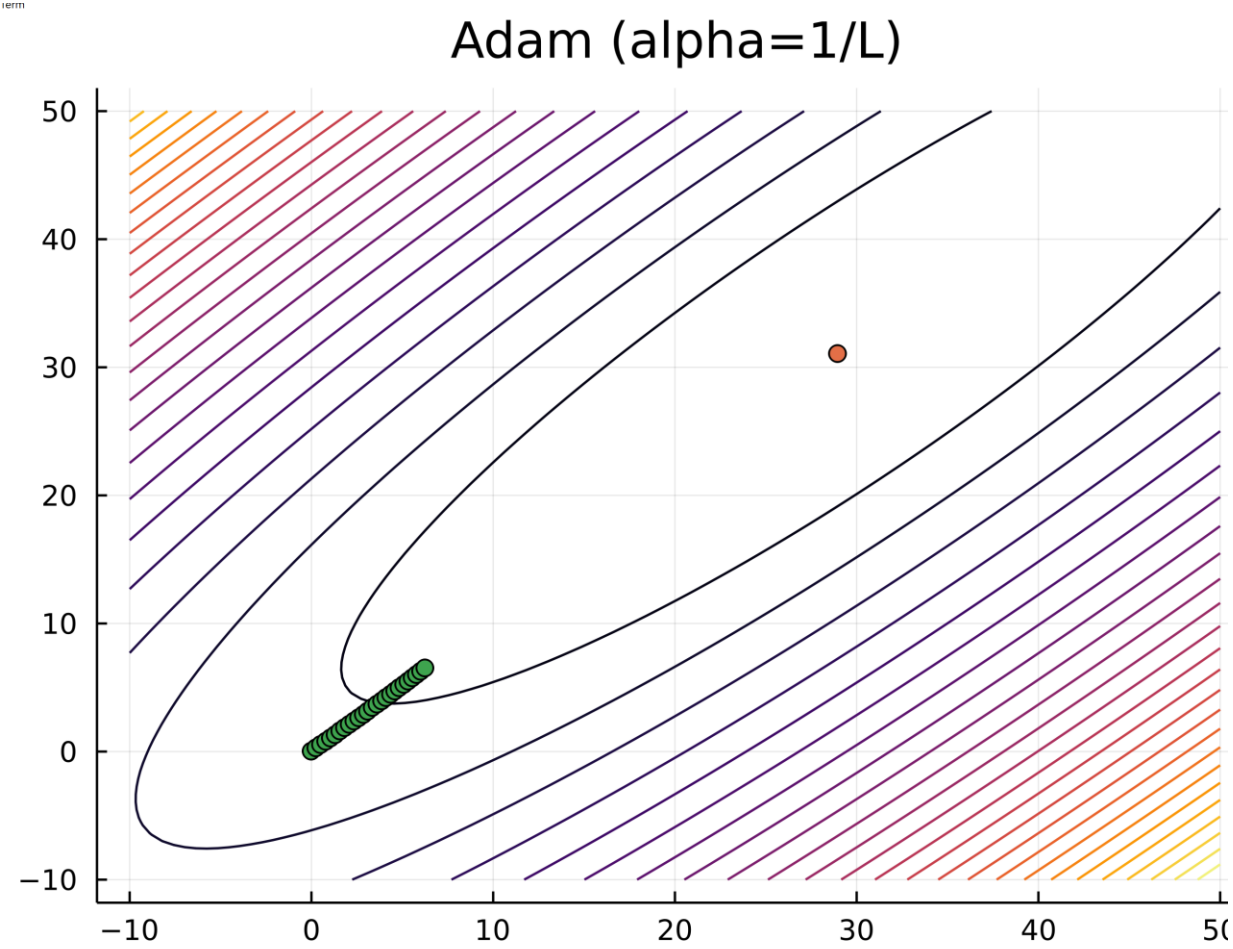




Gradient Descent vs. Adam

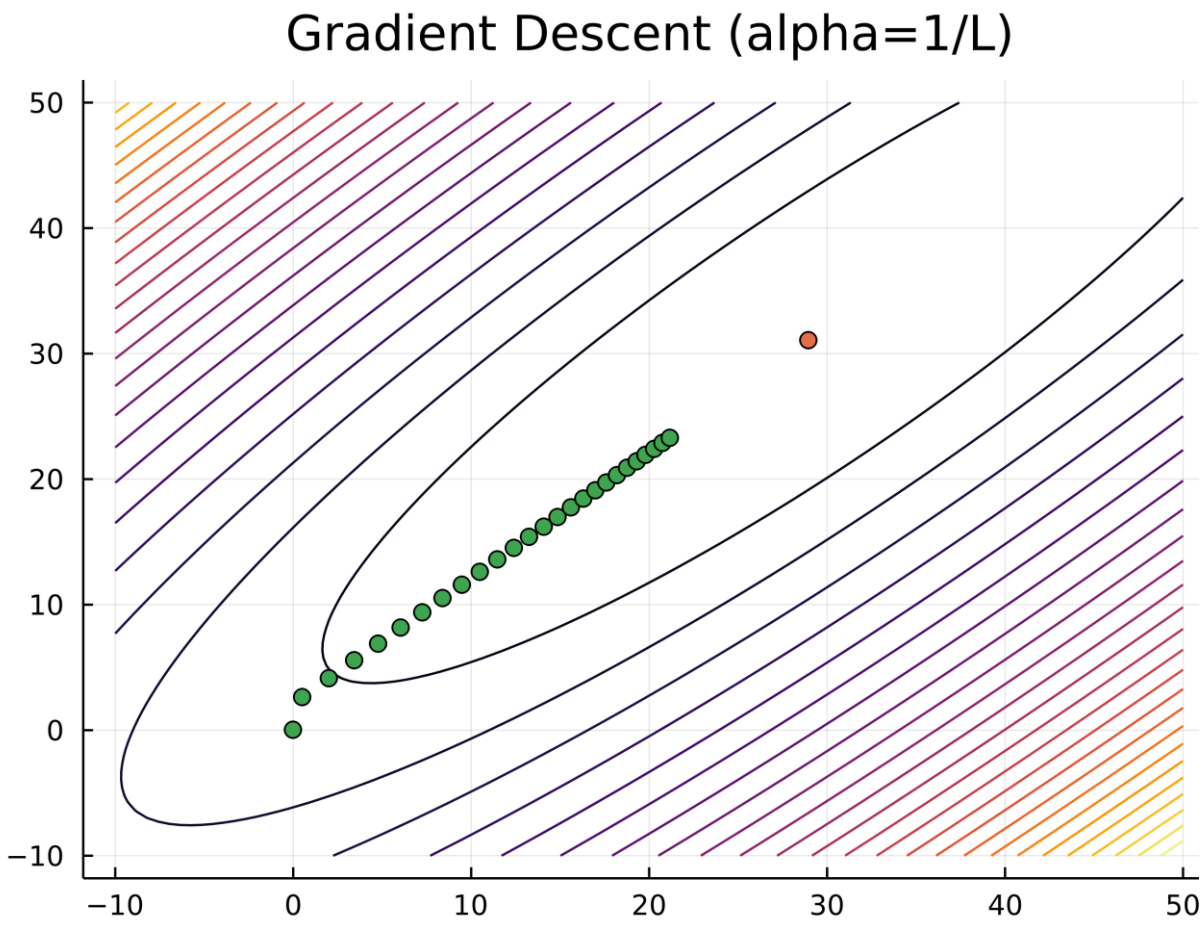
- DGD vs. Adam:

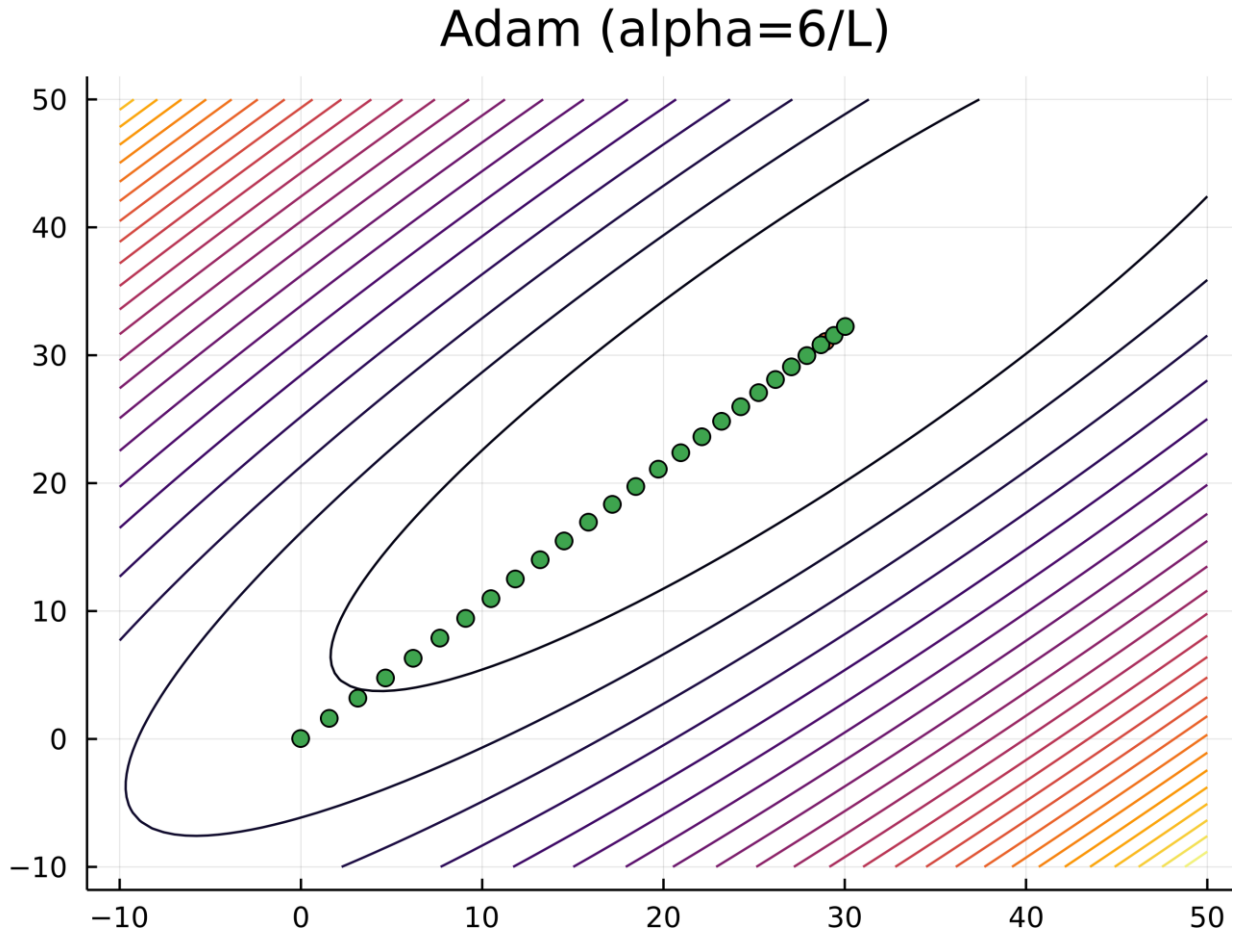




Gradient Descent vs. Adam

- DGD vs. Adam:





Question 7: Should we just use Adam?

- Adam is successful because it better handles heavy-tailed noise?
  - Nope, Adam still outperforms DGD/SGD on neural nets if you remove the noise.

- Adam is successful because we usually apply it to low-noise problems?
  - Nope, Adam can still perform badly on over-parameterized problems.
    - And it works great on some problems that are under-parameterized.

- Adam has more hyper-parameters to search over?
  - Nope, many people just use the default parameters.

- We co-evolved networks architectures with Adam?
  - We have "converged" to architectures that happen to be well-suited for Adam?
    - Would explain abnormally good performance of default parameters.
  - If so, what are the properties that make it well-suited?

- Batch normalization is another common method with missing theory.
  - Though there are many recent papers on this topic.

Summary: The Questions vs. Over-Parameterization

- Answers to our questions depend on if you are over-parameterized.
- Question 1: How do I set the step size?
  - Bigger is better, but make sure $\alpha_k < 2/L$ and $||\nabla f(w_k)||^2 < \alpha_k \sigma_k^2$.
  - Constant or line-search for over-parameterized, decreasing and slow convergence for under-parameterized.
- Question 2: How I pick the mini-batch size?
  - Bigger is better, if it does not increasing the iteration cost.
  - Growing batch sizes makes under-parameterized look like over-parameterized.
- Question 3: Should I use variance reduction?
  - No for over-parameterized, yes for under-parameterized.
- Question 4: What about random shuffling?
  - Very likely a good idea.
- Question 5: Should I use importance sampling?
  - Yes for over-parameterized, no for under-parameterized.
- Question 6: Are there faster algorithms?
  - Yes for over-parameterized, no for under-parameterized.
- Question 7: Should we just use Adam?
  - Maybe, I have more questions than answers here.