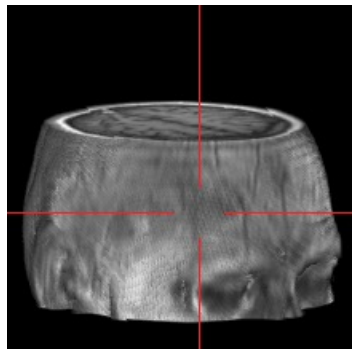
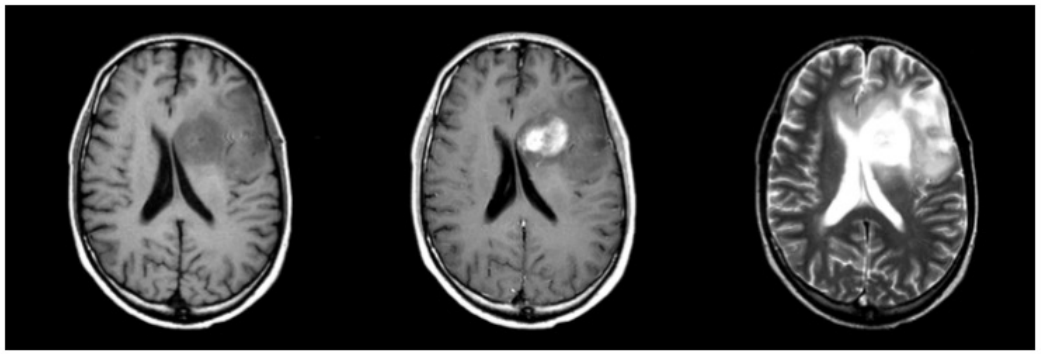
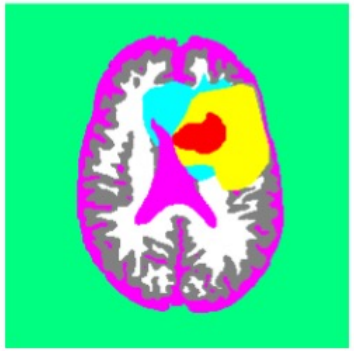
CPSC 340:
Machine Learning and Data Mining

Stochastic Gradient

Spring 2022 (2021W2)

Motivation: Big-N Problems

- Recall the automatic brain tumour segmentation problem:

- MRI scanners at the time produced 200x200x200 volumes.
  - So one volume givens 8 million training examples.
  - And you need to train on more than one volume!

- Similar issues arise in the Gmail application:
  - If every e-mail is a training example, you have LOTS of training examples.

Motivation: Big-N Problems

- Consider fitting a least squares model:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2$$

- Gradient methods are effective when 'd' is very large.
  - O(nd) per iteration instead of $O(nd^2 + d^3)$ to solve as linear system.

- But what if number of training examples 'n' is very large?
  - All Gmails, all products on Amazon, all homepages, all images, etc.

Gradient Descent vs. Stochastic Gradient

- Recall the gradient descent algorithm:

$$w^{t+1} = w^t - \alpha^t \nabla f(w^t)$$

- For least squares, our gradient has the form:

$$\nabla f(w) = \sum_{i=1}^{n} (w^T x_i - y_i) x_i$$

(scalar; $d \times 1$)

- So the cost of computing this gradient is linear in 'n'.
  - As 'n' gets large, gradient descent iterations become expensive.

Gradient Descent vs. Stochastic Gradient

- Common solution to this problem is stochastic gradient algorithm:

$$w^{t+1} = w^t - \alpha^t \nabla f_i(w^t)$$

- Uses the gradient of a randomly-chosen training example:

$$\nabla f_i(w) = (\underbrace{w^T x_i - y_i}_{\text{scalar}}) \underbrace{x_i}_{d \times 1}$$

- Cost of computing this one gradient is independent of 'n'.
  - Iterations are 'n' times faster than gradient descent iterations.
  - With 1 billion training examples, this iteration is 1 billion times faster.

Stochastic Gradient (SG)

- Stochastic gradient is an iterative optimization algorithm:
  - We start with some initial guess, w^0.
  - Generate new guess by moving in the negative gradient direction:

$$w^1 = w^0 - \alpha^0 \nabla f_i(w^0)$$

    - For a random training example 'i'.
  - Repeat to successively refine the guess:

$$w^{t+1} = w^t - \alpha^t \nabla f_i(w^t) \quad \text{for } t = 1, 2, 3, \ldots$$

    - For a random training example 'i'.

Problem where we can use Stochastic Gradient

- Stochastic gradient applies when minimizing averages:

$$f(w) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2 \quad \text{(squared error)}$$

$$f(w) = \frac{1}{n}\sum_{i=1}^{n}\log(1+\exp(-y_i w^T x_i)) \quad \text{(logistic regression)}$$

$$f(w) = \frac{1}{n}\sum_{i=1}^{n}\left[\log(1+\exp(-y_i w^T x_i)) + \frac{\lambda}{2}\|w\|^2\right] \quad (L_2\text{-regularized logistic})$$

$$f(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w) \quad \text{(our notation for the general case)}$$

- Basically, all our regression losses except "brittle" regression.
  - Recall: multiplying by positive constant doesn't change location of optimal 'w'.

Why Does Stochastic Gradient Work / Not Work?

- Main problem with stochastic gradient:
  - Gradient of random example might point in the wrong direction.

- Does this have any hope of working?
  - The expected direction is the full gradient.

$$E[\nabla f_i(w^k)] = \sum_{i=1}^{n} p(i)\nabla f_i(w^k) = \sum_{i=1}^{n} \frac{1}{n}\nabla f_i(w^k) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(w^k) = \nabla f(w^k)$$

expectation over choice of random example i

definition of expectation

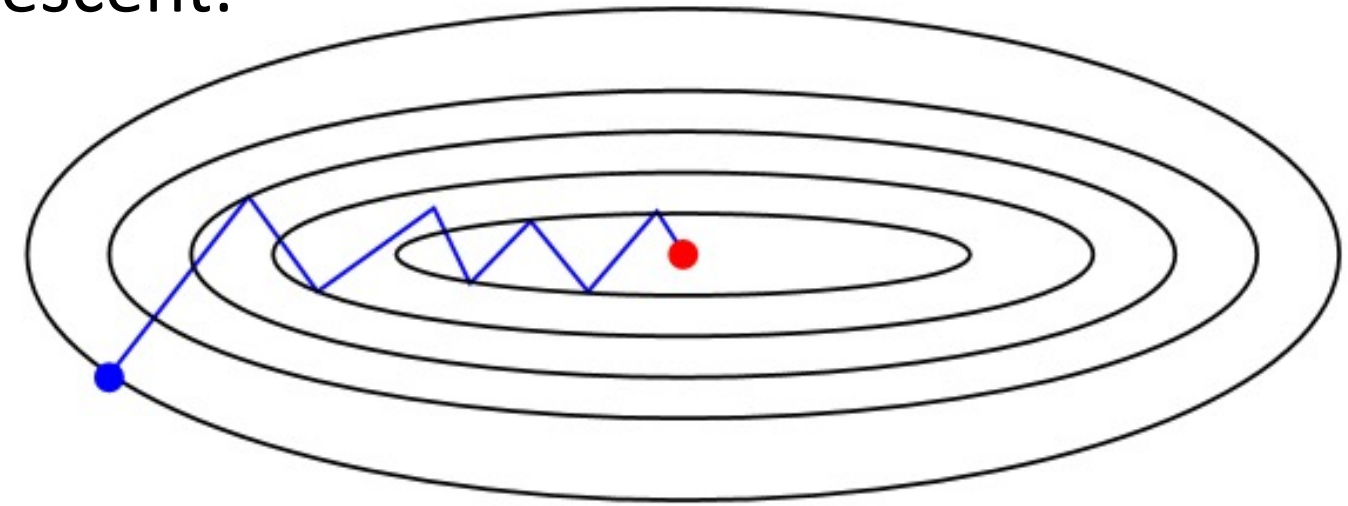
if each example is equally likely

gradient over all examples

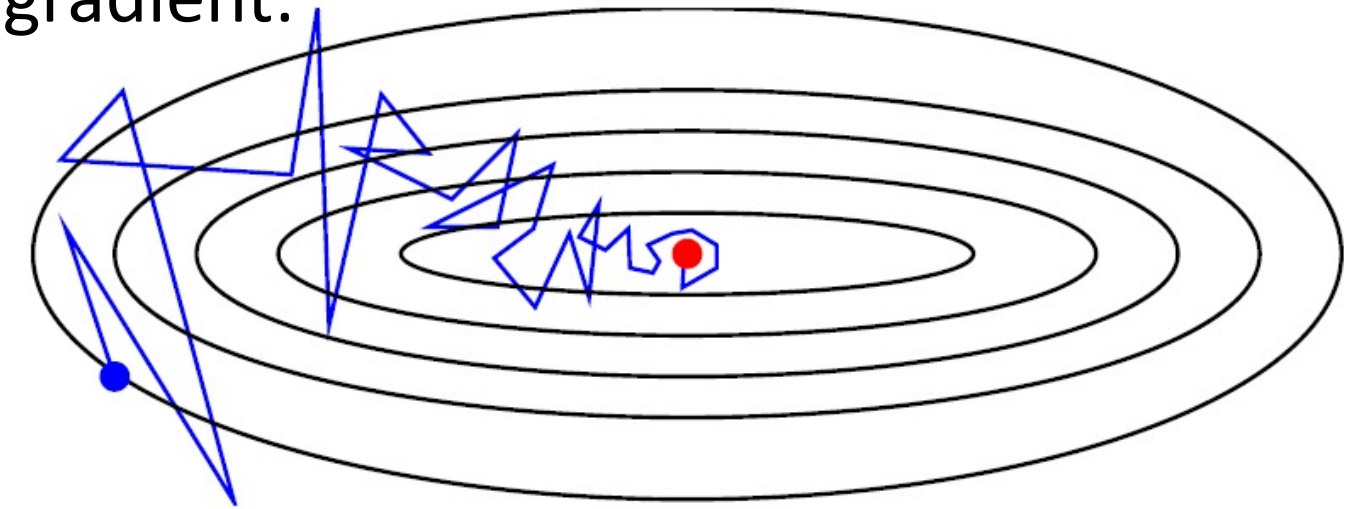
  - The algorithm is going in the right direction on average.

Gradient Descent vs. Stochastic Gradient (SG)

- Gradient descent:

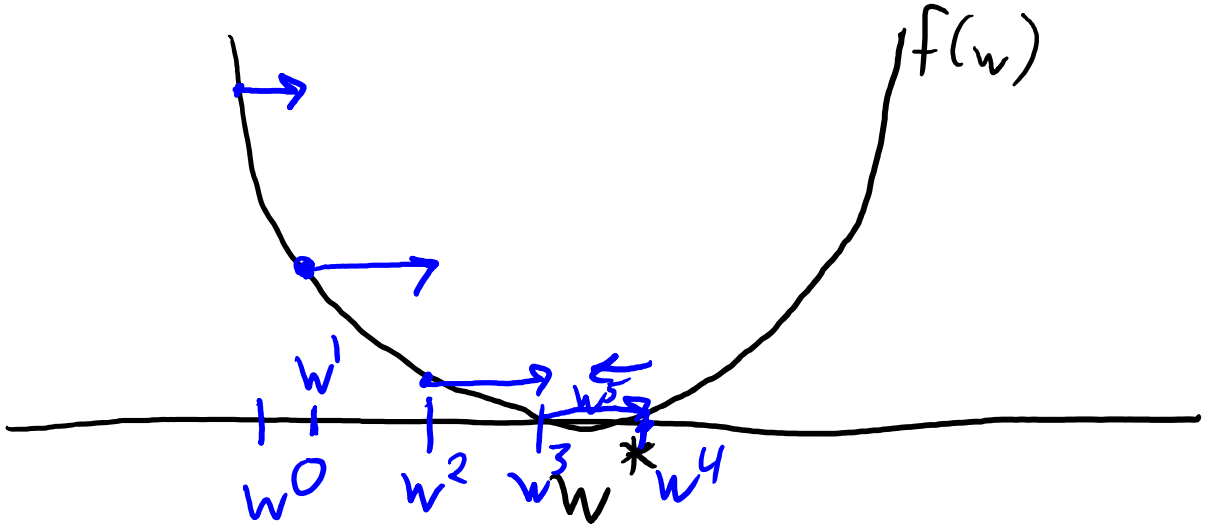


- Stochastic gradient:



Gradient Descent in Action

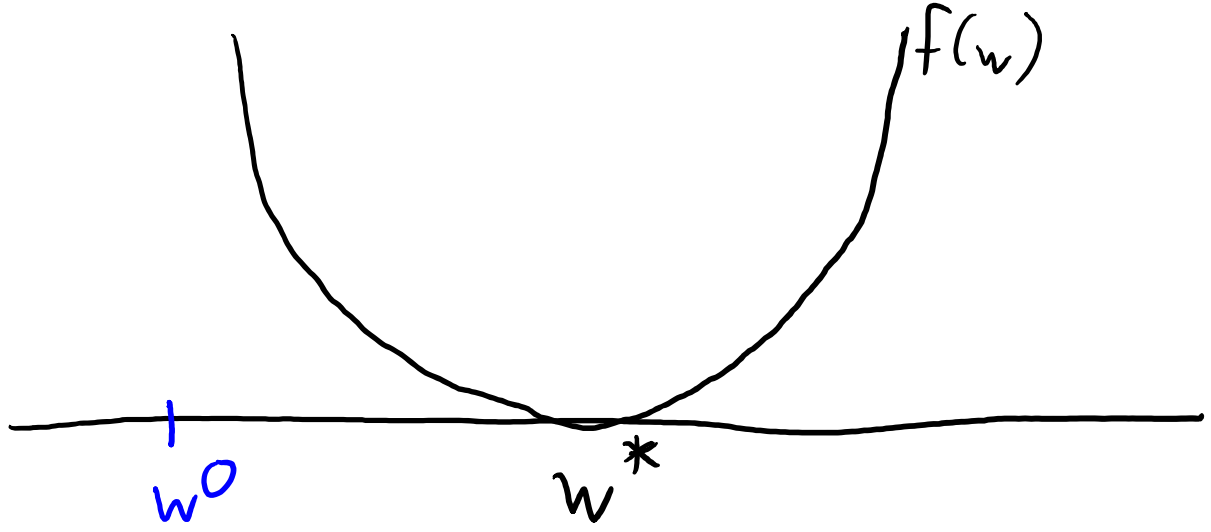
$$f(w) = \frac{1}{5}\sum_{i=1}^{5} (w^T x_i - y_i)^2$$

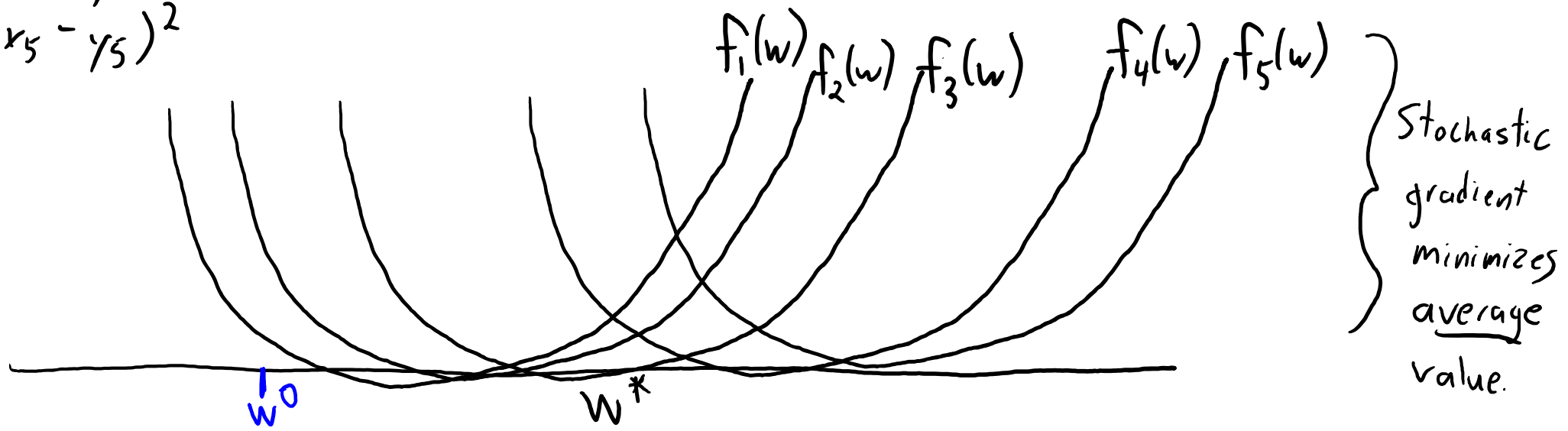


Stochastic Gradient in Action

$$f(w) = \frac{1}{5}\sum_{i=1}^{5} (w^T x_i - y_i)^2$$

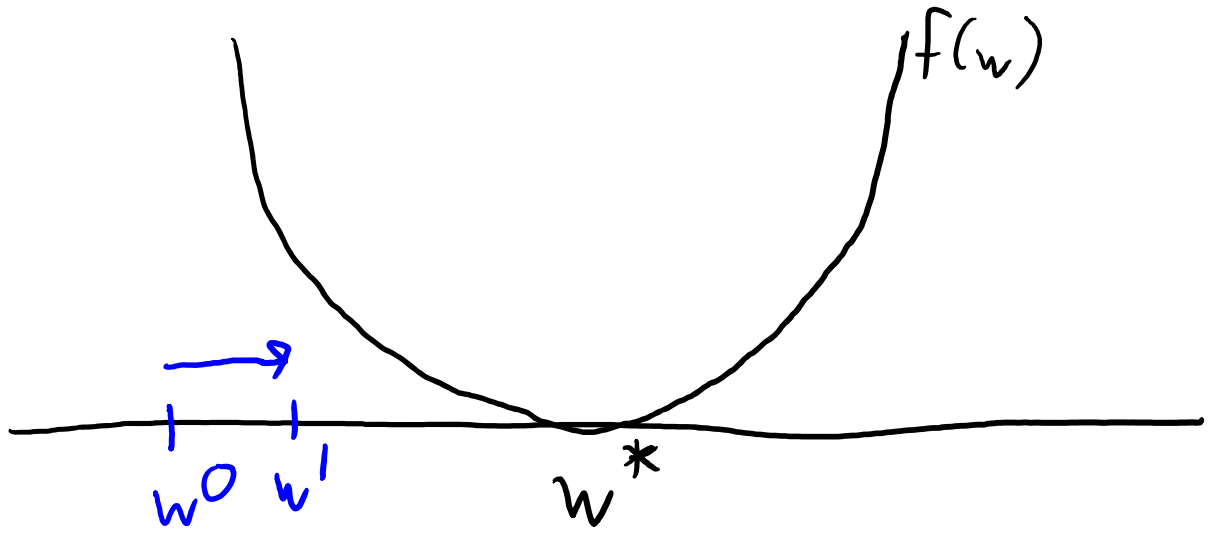
$$f_1(w) = (w^T x_1 - y_1)^2$$
$$f_2(w) = (w^T x_2 - y_2)^2$$
$$f_3(w) = (w^T x_3 - y_3)^2$$
$$f_4(w) = (w^T x_4 - y_4)^2$$
$$f_5(w) = (w^T x_5 - y_5)^2$$

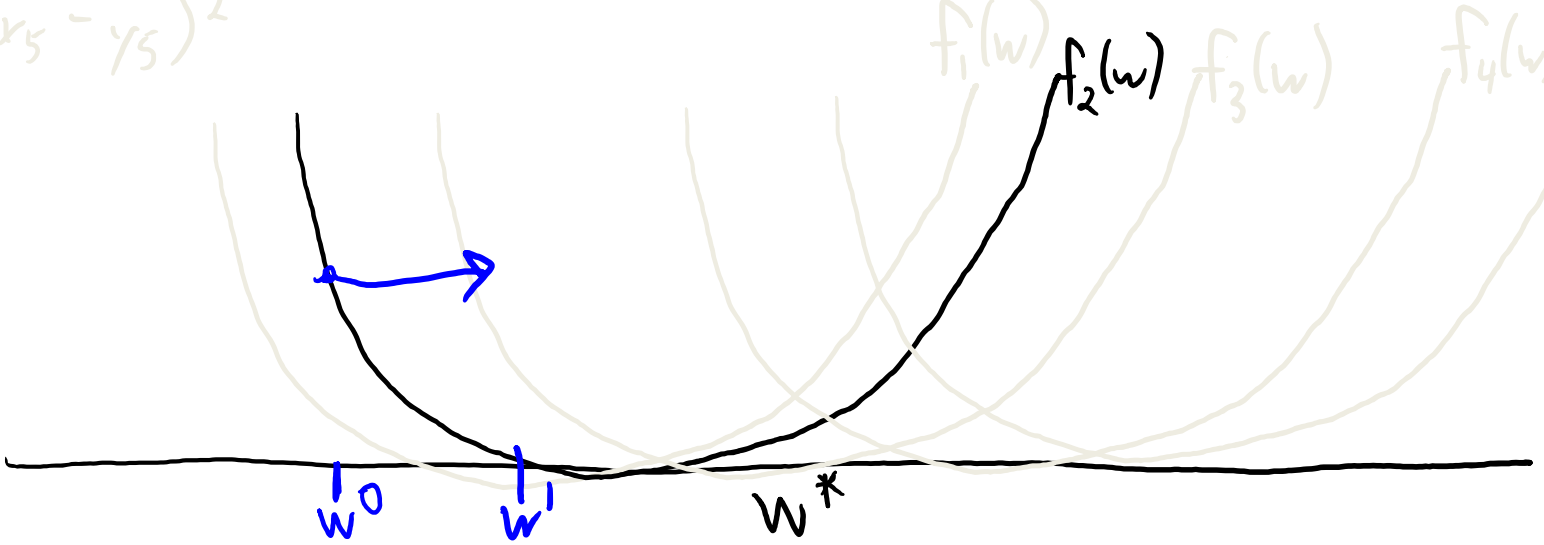




Stochastic Gradient in Action

$$f_2(w) = (w^T x_2 - y_2)^2$$

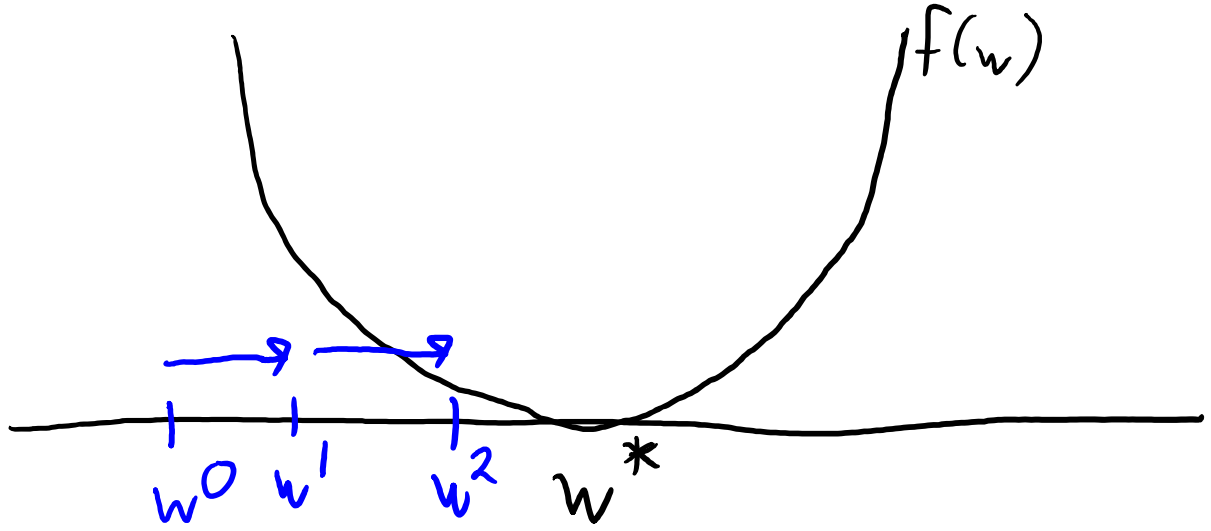


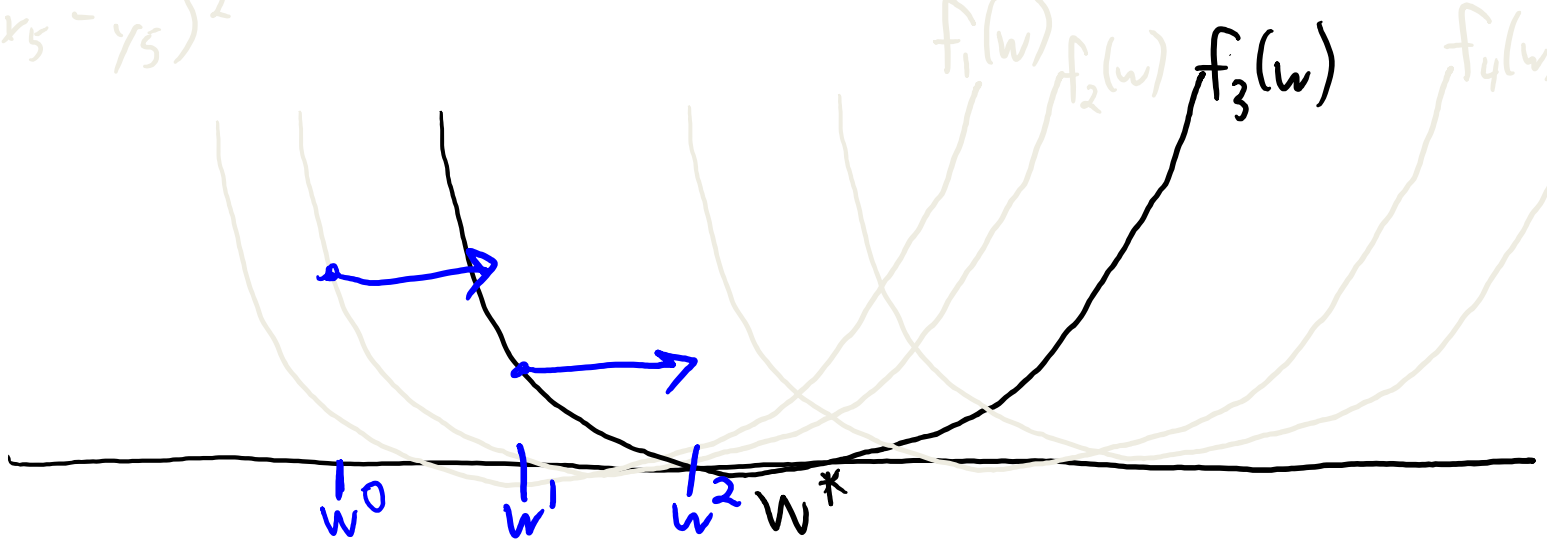


Stochastic gradient minimizes average value.

Stochastic Gradient in Action

$$f_3(w) = (w^T x_3 - y_3)^2$$





Stochastic gradient minimizes average value.

Stochastic Gradient in Action

$$f(w) = \frac{1}{5}\sum_{i=1}^{5} (w^T x_i - y_i)^2$$

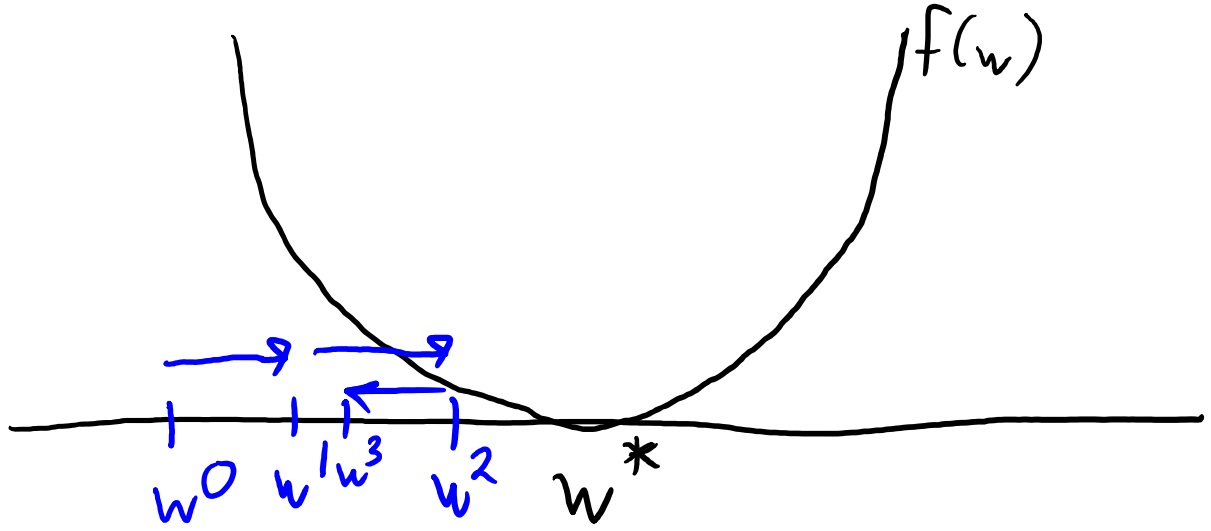
$$f_1(w) = (w^T x_1 - y_1)^2$$

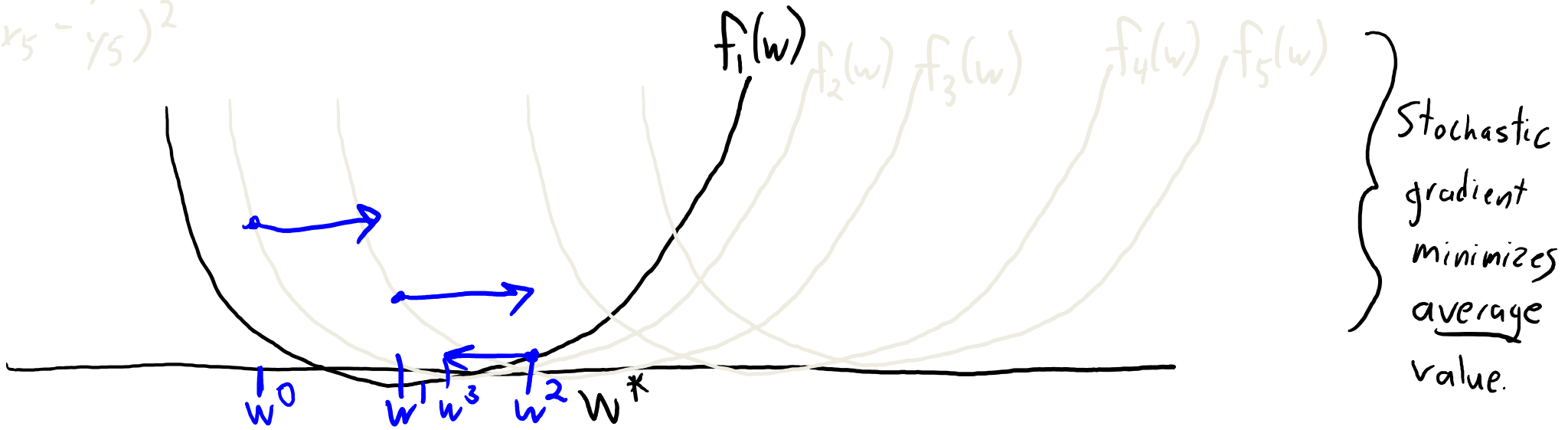
$$f_2(w) = (w^T x_2 - y_2)^2$$

$$f_3(w) = (w^T x_3 - y_3)^2$$

$$f_4(w) = (w^T x_4 - y_4)^2$$

$$f_5(w) = (w^T x_5 - y_5)^2$$





Stochastic gradient minimizes average value.

Stochastic Gradient in Action

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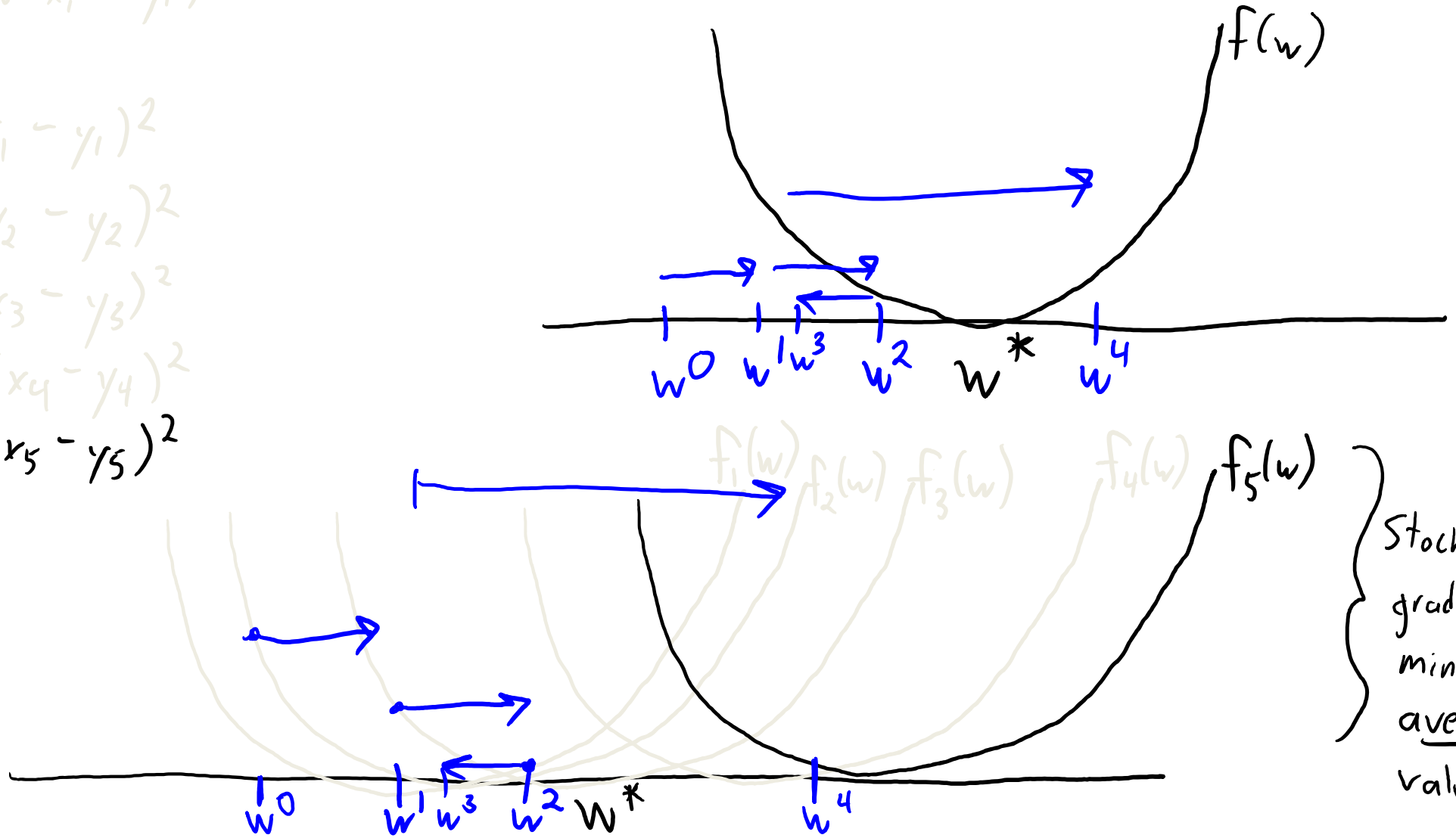
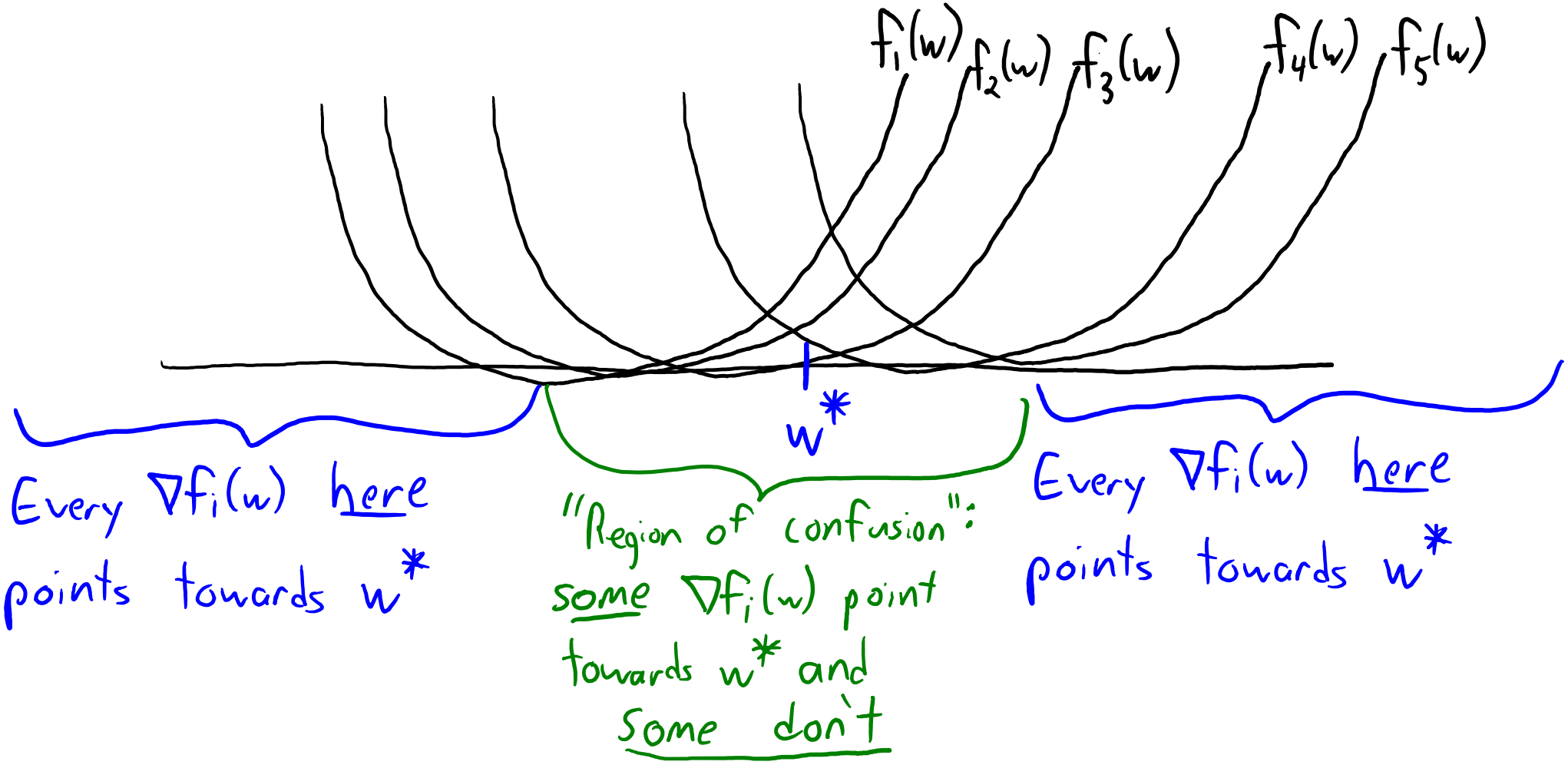
$$f_5(w) = (w^T x_5 - y_5)^2$$



Effect of 'w' Location on Progress



- We'll still make good progress if most gradients points in right direction.

Variance of the Random Gradients

- The "confusion" is captured by a kind of variance of the gradients:

$$\frac{1}{n}\sum_{i=1}^{n} \|\nabla f_i(w^t) - \nabla f(w^t)\|^2$$

gradient of example i — average gradient over all examples

- If the variance is 0, every step goes in the right direction.
  - We're outside of the region of confusion.
- If the variance is small, most steps point in the direction.
  - We're just inside region of confusion.
- If the variance is large, many steps will point in the wrong direction.
  - Middle of region of confusion, where w^* lives.

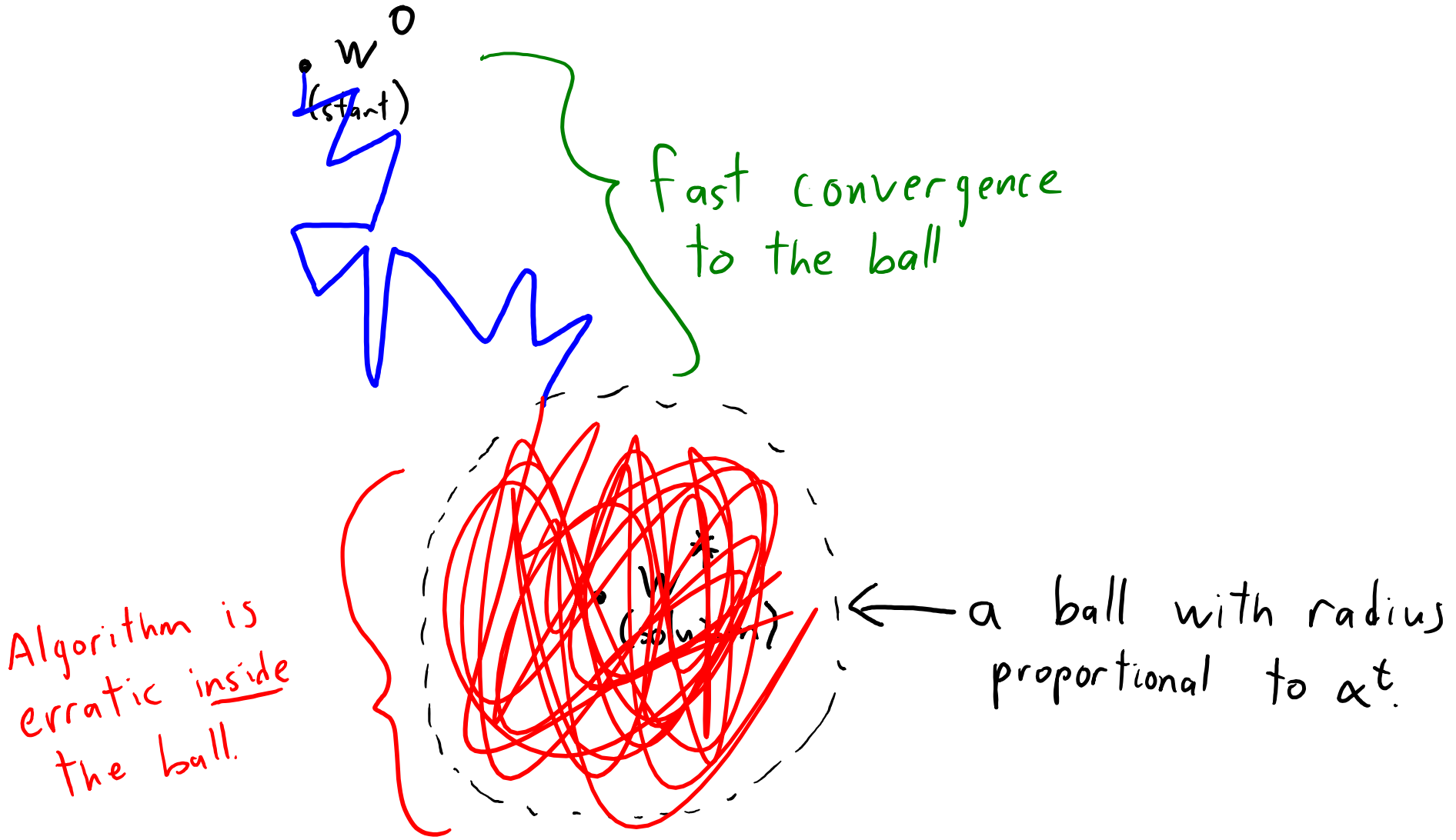
Effect of the Step-Size

- We can reduce the effect of the variance with the step size.
  - Variance slows progress by amount proportional to square of step-size.
  - So as the step size gets smaller, the variance has less of an effect.

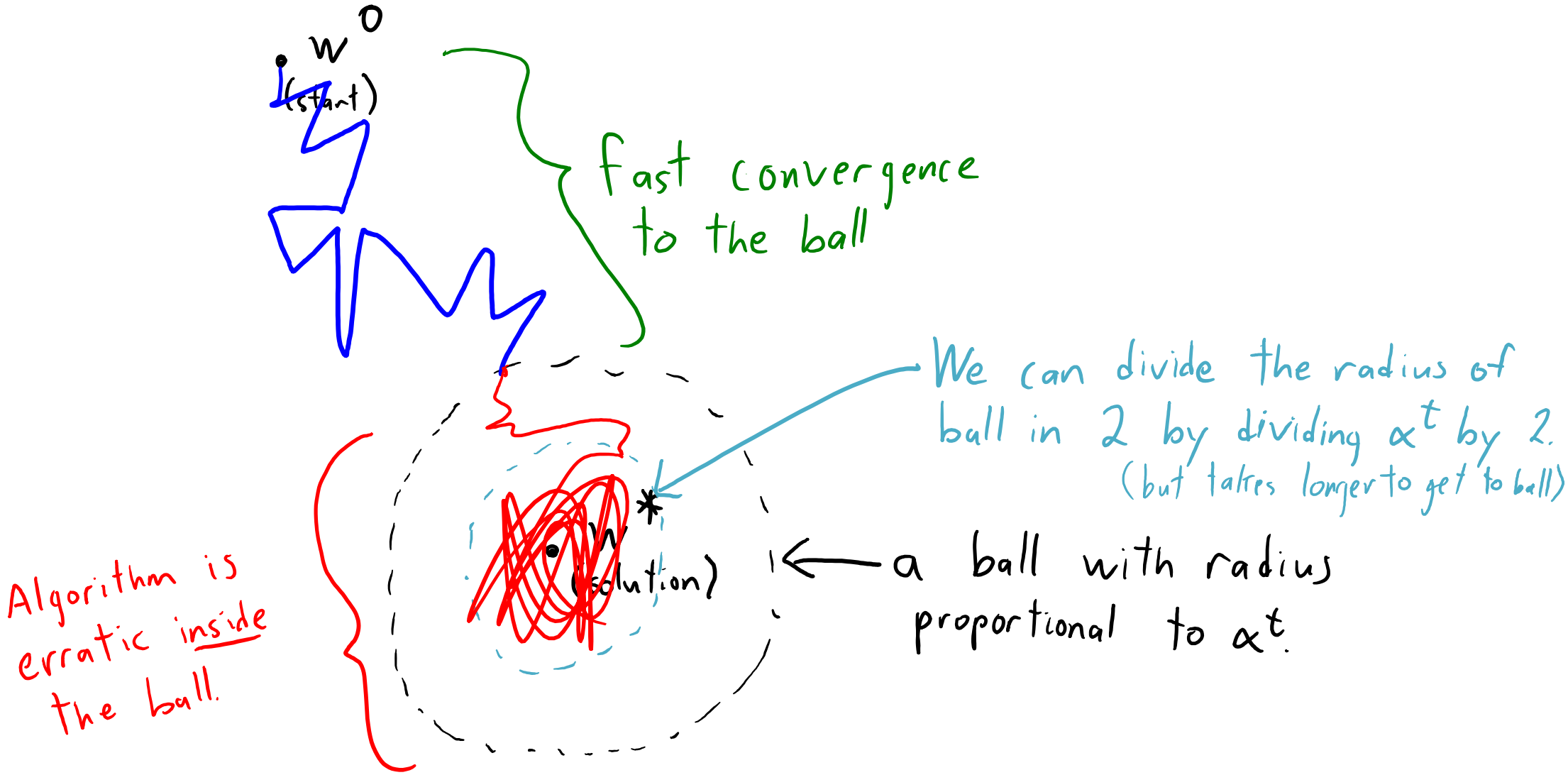
- For a fixed step-size, SG makes progress until variance is too big.

- This leads to two "phases" when we use a constant step-size:
  1. Rapid progress when we are far from the solution.
  2. Erratic behaviour confined to a "ball" around solution.
     (Radius of ball is proportional to the step-size.)

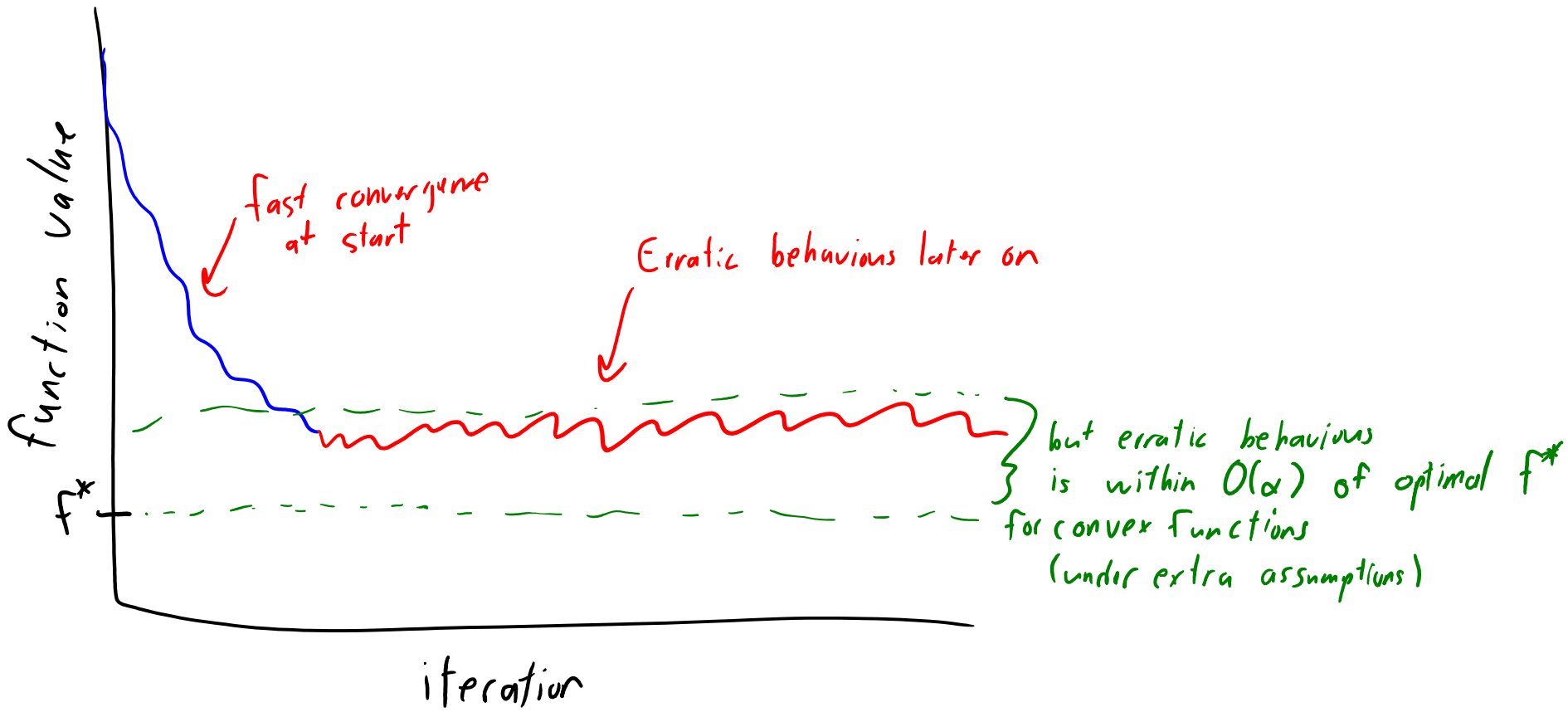
Stochastic Gradient with Constant Step Size



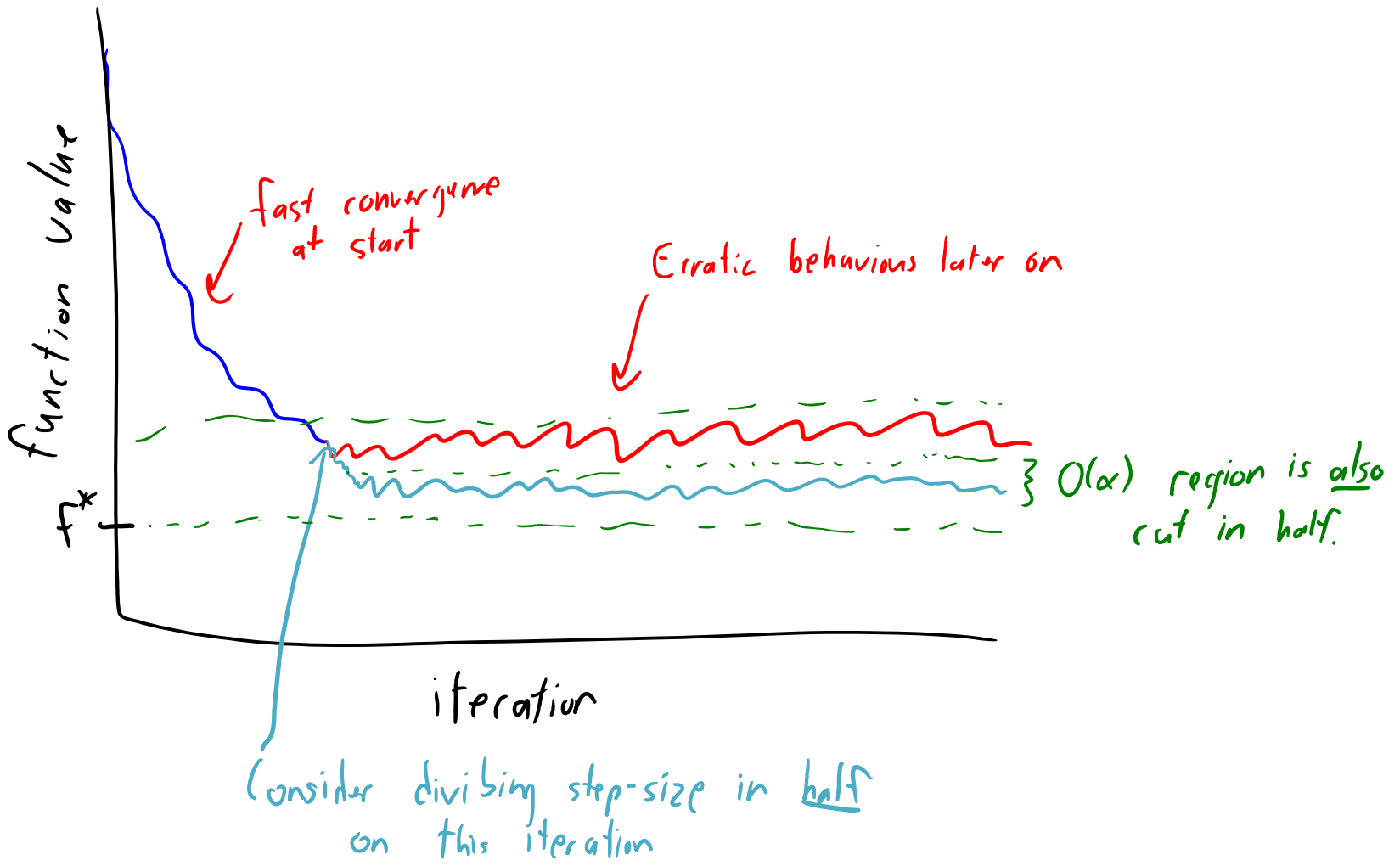
Stochastic Gradient with Constant Step Size



Stochastic Gradient with Constant Step Size



Stochastic Gradient with Constant Step Size



Stochastic Gradient with Decreasing Step Sizes

- To get convergence, we need a decreasing step size.
  - Shrinks size of ball to zero so we converge to w^*.
- But it can't shrink too quickly:
  - Otherwise, we don't move fast enough to reach the ball.
- Stochastic gradient converges to a stationary point if:
  - Ratio of sum of squared step-sizes over sum of step-sizes converges to 0.

"how much noise affects you" → $\sum_{t=1}^{\infty} (\alpha^t)^2$

"how far you can get" → $\sum_{t=1}^{\infty} \alpha^t$

$$\frac{\sum_{t=1}^{\infty} (\alpha^t)^2}{\sum_{t=1}^{\infty} \alpha^t} = 0$$

  - This choice also works for non-smooth funtions like SVMs.
    - Function must be continuous and not "too crazy" (we're still figuring it out for non-convex).

Stochastic Gradient with Decreasing Step Sizes

- For convergence step-sizes need to satisfy: $\sum_{t=1}^{\infty} (\alpha^t)^2 / \sum_{t=1}^{\infty} \alpha^t = 0$

- Classic solution is to use a step-size sequence like $\alpha^t = O(1/t)$.

$$\sum_{t=1}^{\infty} \alpha^t = \sum_{t=1}^{\infty} \frac{1}{t} = \infty$$

"we can get everywhere"

$$\sum_{t=1}^{\infty} (\alpha^t)^2 = \sum_{t=1}^{\infty} \frac{1}{t^2} < \infty$$

"effect of variance goes to zero"

  - E.g., $\alpha^t = .001/t$.
- Unfortunately, this often works badly in practice:
  - Steps get really small really fast.
  - Some authors add extra parameters like $\alpha^t = \gamma/(\beta t + \Delta)$, which helps a bit.
  - One of the only cases where this works well: binary SVMs with $\alpha^t = 1/\lambda t$.

Stochastic Gradient with Decreasing Step Sizes

- How do we pick step-sizes satisfying $\sum_{t=1}^{\infty} (\alpha^t)^2 / \sum_{t=1}^{\infty} \alpha^t = 0$

- Better solution is to use a step-size sequence like $\alpha^t = O(1/\sqrt{t})$.

$$\sum_{t=1}^{k} \alpha^t = \sum_{t=1}^{k} \frac{1}{\sqrt{t}} = O(\sqrt{k}) \qquad \sum_{t=1}^{k} (\alpha^t)^2 = \sum_{t=1}^{k} \frac{1}{t} = O(\log k)$$

  - E.g., use $\alpha^t = .001/\sqrt{t}$
  - Both sequences diverge, but denominator diverges faster.

- This approach (roughly) optimizes rate that ratio goes to zero.
  - Better worst-case theoretical properties (and more robust to step-size).
  - Often better in practice too.

Stochastic Gradient with Constant Step Sizes?

- Alternately, could we just use a constant step-size?
  - E.g., use $\alpha^t = .001$ for all 't'.
- This will not converge to a stationary point in general.
  - However, do we need it to converge?
- What if you only care about the first 2-3 digits of the test error?
  - Who cares if you aren't able to get 10 digits of optimization accuracy?
- There is a step-size small enough to achieve any fixed accuracy.
  - Just need radius of "ball" to be small enough.

Mini-batches: Using more than 1 example

bonus!

- Does it make sense to use more than 1 random example?
  - Yes, you can use a "mini-batch" B^t of examples.

$$w^{t+1} = w^t - \alpha^t \frac{1}{|B^t|} \sum_{i \in B^t} \nabla f_i(w^t)$$

Random "batch" of examples.

  - Radius of ball is inversely proportional to the mini-batch size.
    - If you double the batch size, you half the radius of the ball.
      - Big gains for going from 1 to 2, less big gains from going from 100 to 101.
    - You can use a bigger step size as the batch size increases ("linear scaling" rule).
      - Gets you to the ball faster (though diverges if step-size gets too big).
  - Useful for vectorizing/parallelizing code.
    - Evaluate one gradient on each core.

bonus!

Random vs. Re-shuffle SGD

- Classic SGD: i_k sampled randomly "with replacement".
- SGD with "random shuffling":
  - Generate a random ordering of the example 1,2,…,n.
  - Do an SGD step on each example, following the random order.
    - Sampling "without replacement".
  - Go back to step 1.
- We used to view this as an "engineering trick".
  - You can speed up the code by ordering examples in memory.
    - Variation 1: always use the same shuffle (only do step 1 once).
    - Variation 2: alternate between two shuffles.
- We now know that random shuffling converges faster in many cases.
  - Took a long time to prove: as stochastic gradients are biased and dependent.

bonus!

Polyak-Ruppert Iterate Averaging

- Another practical/theoretical trick is averaging of the iterations.
  1. Run the stochastic gradient algorithm with $\alpha^t = O(1/\sqrt{t})$ or α^t constant.
  2. Take some weighted average of the w^t values.

$$\bar{w}^t = \sum_{k=1}^{t} v^k w^k$$

Here, v^k is a scalar "weight" of iteration 'k'

Uniform average:

$$\bar{w}^t = \frac{1}{t} \sum_{k=1}^{t} w^k$$

$v^k = \frac{1}{t}$

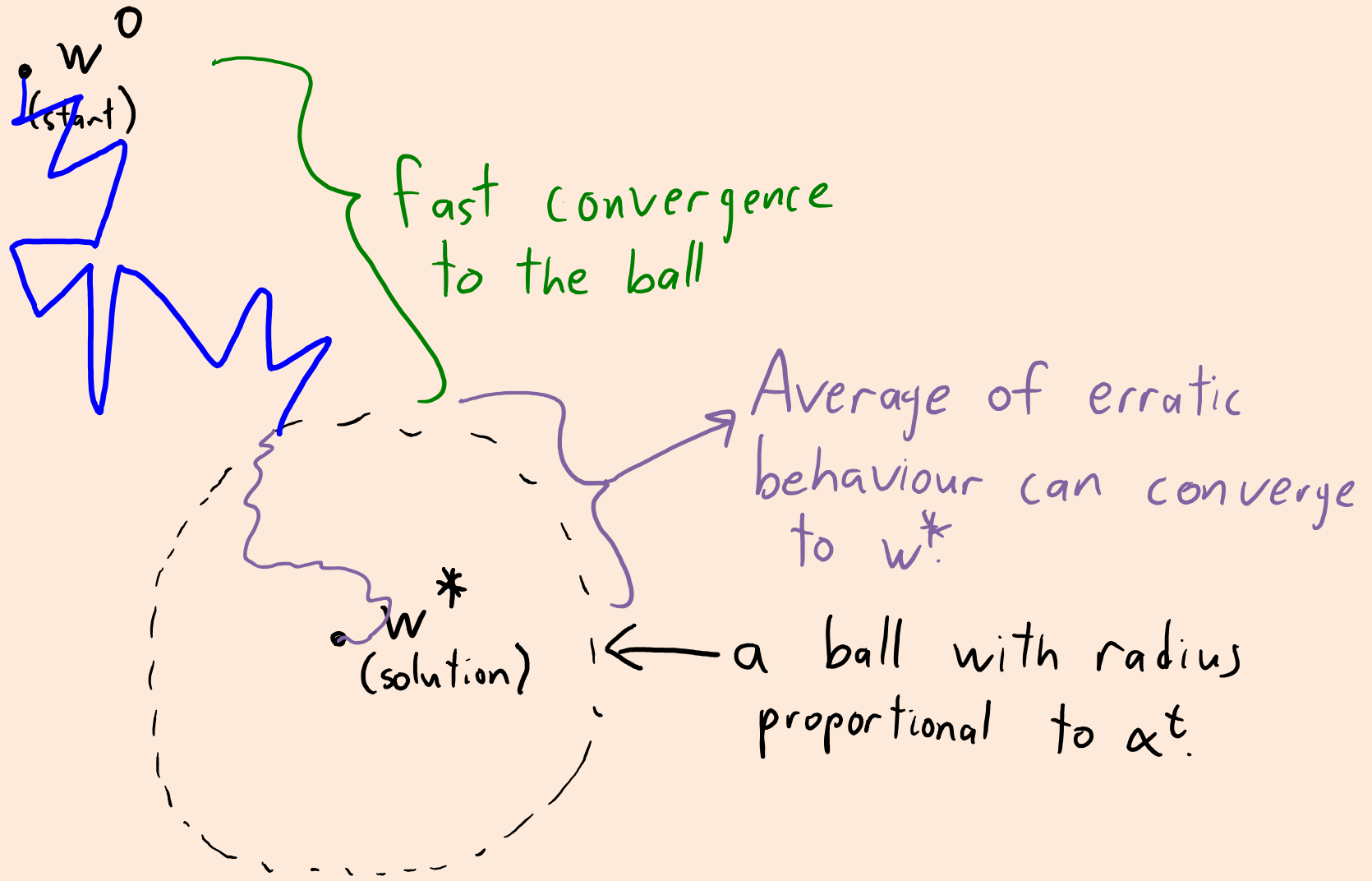
- Average does not affect the algorithm, it's just "watching".
- Surprising result shown by Polyak and by Ruppert in the 1980s:
  - Asymptotically converges as fast as stochastic Newton's method.

bonus!

Stochastic Gradient with Averaging

Often, you average the second half of the iterations.

Set $\bar{w}^t = \frac{1}{t/2} \sum_{k=t/2}^{t} w^k$



A Practical Strategy for Deciding When to Stop

- In gradient descent, we can stop when gradient is close to zero.

- In stochastic gradient:
  - Individual gradients don't necessarily go to zero.
  - We can't see full gradient, so we don't know when to stop.

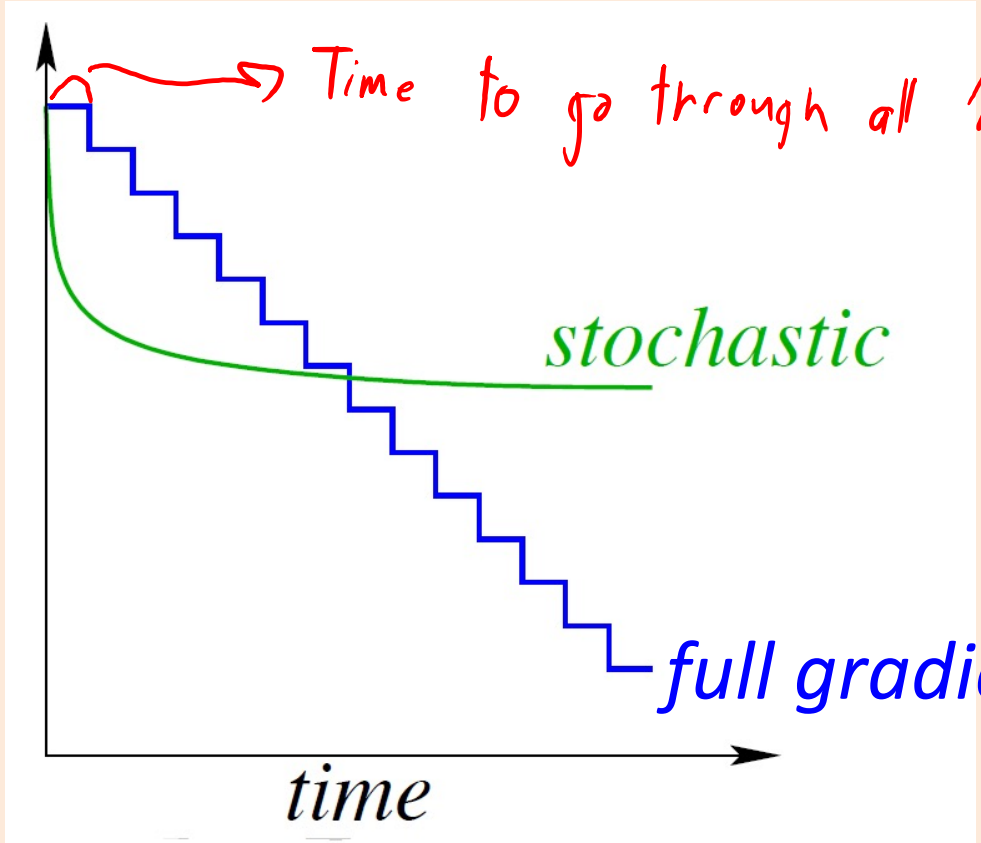
- Practical trick:
  - Every 'k' iterations (for some large 'k'), measure validation set error.
  - Stop if the validation set error "isn't improving".
    - We don't check the gradient, since it takes a lot longer for the gradient to get small.
    - This "early stopping" can also reduce overfitting.

Summary

- Step-size in stochastic gradient is a huge pain:
  - Needs to go to zero to get convergence, but classic O(1/t) steps are bad.
  - $O(1/\sqrt{t})$ works better, but still pretty slow.
  - Constant step-size is fast, but only up to a certain point.
- Bonus slides summary
  - SGD practical issues: mini-batching, averaging, termination.
  - SAG and other methods fix SG convergence for finite datasets.
  - Infinite datasets can be used with SG and do not overfit.

bonus!

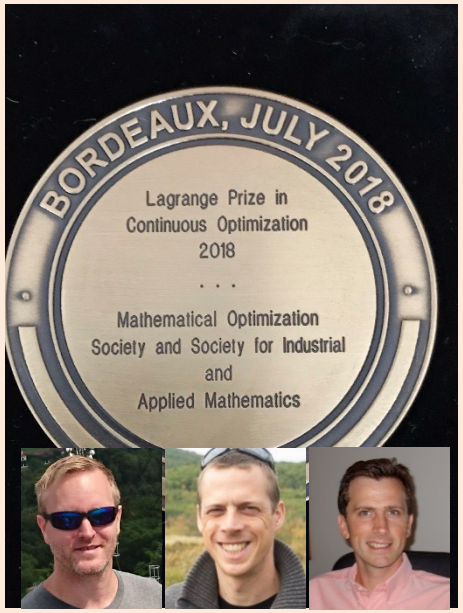
Gradient Descent vs. Stochastic Gradient



- 2012: methods with cost of stochastic gradient, progress of full gradient.
  - Key idea: if 'n' is finite, you can use a memory instead of having α_t go to zero.
  - First was stochastic average gradient (SAG), "low-memory" version is SVRG.

bonus!

This graph shows how algorithms have become fast and more efficient over time. The horizontal axis represents time and the vertical axis represents error. Older algorithms (yellow) were very slow but had very little error. Faster algorithms were created by only analyzing some of the data (orange). The method was faster but had an accuracy limit. Schmidt's algorithm is faster and has no accuracy limit. *Aiken Lao / The Ubyssey*

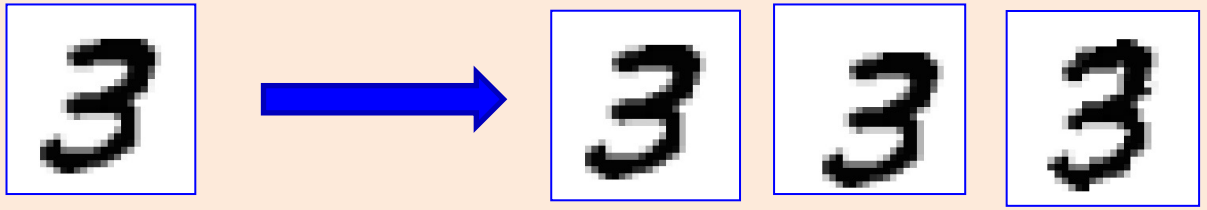


https://www.ubyssey.ca/science/schmidt-sloan-fellowship/

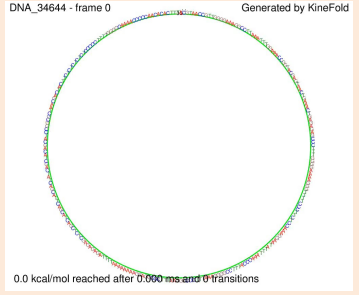
bonus!

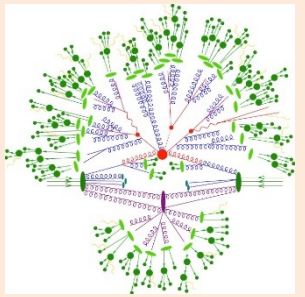
Machine Learning with “n = ∞”

- Here are some scenarios where you effectively have “n = ∞”:
  - A dataset that is so large we cannot even go through it once (Gmail).
  - A function you want to minimize that you can’t measure without noise.
  - You want to encourage invariance with a continuous set of transformation:
    - You consider infinite number of translations/rotations instead of a fixed number.



  - Learning from simulators with random numbers (physics/chem/bio):





http://kinefold.curie.fr/cgi-bin/form.pl
https://sciencenode.org/feature/sherpa-and-open-science-grid-predicting-emergence-jets.php

bonus!

Stochastic Gradient with Infinite Data

- Previous slide gives examples with infinite sequence of IID samples.
- How can you practically train on infinite-sized datasets?
- Approach 1 (exact optimization on finite 'n'):
  - Grab 'n' data points, for some really large 'n'.
  - Fit a regularized model on this fixed dataset ("empirical risk minimization").
- Approach 2 (stochastic gradient for 'n' iterations):
  - Run stochastic gradient iteration for 'n' iterations.
  - Each iteration considers a new example, never re-visiting any example.

bonus!

Stochastic Gradient with Infinite Data

- Approach 2 works because of an amazing property of stochastic gradient:
  - The classic convergence analysis does not rely on 'n' being finite.

- Further Approach 2 only looks at a data point once:
  - Each example is an unbiased approximation of test data.
- So Approach 2 is doing stochastic gradient on test error:
  - It cannot overfit.

- Up to a constant, Approach 1 and 2 have same test error bound.
  - This is sometimes used to justify SG as the "ultimate" learning algorithm.
    - "Optimal test error by computing gradient of each example once!"
  - In practice, Approach 1 usually gives lower test error.
    - The constant factor matters!

bonus!

A Practical Strategy For Choosing the Step-Size

- All these step-sizes have a constant factor in the "O" notation.
  - E.g., $\alpha^t = \frac{\gamma}{\sqrt{t}}$ ← How do we choose this constant?

- We don't know how to set step size as we go in the stochastic case.
  - And choosing wrong γ can destroy performance.

- Common practical trick:
  - Take a small amount of data (maybe 5% of the original data).
  - Do a binary search for γ that most improves objective on this subset.