» Stochastic Gradient Descent (SGD)

* Recall our general iterative minimisation algorithm:

```
x=x0
for k in range(num_iters):
    step = calcStep(fn,x)
    x = x - step
```

and one way to choose the step, namely:

$$step = \alpha[\frac{\partial f}{\partial x_1}(x), \frac{\partial f}{\partial x_2}(x), \ldots, \frac{\partial f}{\partial x_n}(x)]$$

* We've spent a good deal of time looking at how to select step-size/learning rate α
* Now let's go back and look at how we calculate $\frac{\partial f}{\partial x_1}(x)$ etc

» Approximate Derivatives

* $f(x) \approx f(x') + \frac{\partial f}{\partial x_1}(x')(x_1 - x'_1) + \frac{\partial f}{\partial x_2}(x')(x_2 - x'_2) + \cdots + \frac{\partial f}{\partial x_n}(x')(x_n - x'_n)$
* Choosing x with $x_1 = x' - \alpha \frac{\partial f}{\partial x_1} x')$, $x_2 = x' - \alpha \frac{\partial f}{\partial x_2} x')$, $\ldots$, $x_n = x' - \alpha \frac{\partial f}{\partial x_n} x')$ then

$$f(x) \approx f(x') - \alpha \frac{\partial f}{\partial x_1}(x')^2 - \alpha \frac{\partial f}{\partial x_2}(x')^2 - \cdots - \alpha \frac{\partial f}{\partial x_n}(x')^2$$

  i.e. moving from point x' to x tends to decrease function $f(\cdot)$
* This is already an approximation, so why not also use an approximation to the derivative i.e.

$$x_1 = x' - \alpha Df_{x_1}(x'), \ \textit{etc}$$

  with $Df_{x_1}(x') \approx \frac{\partial f}{\partial x_1}(x')$, etc

» Approximate Derivatives

* Let's swap from $\min_x f(x)$ to $\min_\theta J(\theta)$ to be consistent with our ML notation. Functions we want to minimise in ML are often of the form:

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} loss(\theta, x^{(i)}, y^{(i)})$$

where

* $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$ is our training data
* $loss()$ is a function that measures how well our predictions match the training data
  e.g. $loss(\theta, , x^{(i)}, y^{(i)}) = (\theta^T x^{(i)} - y^{(i)})^2$ in linear regression
* Derivatives:

$$\frac{\partial J}{\partial \theta_1}(\theta) = \frac{1}{m}\sum_{i=1}^{m} \frac{\partial loss}{\partial \theta_1}(\theta, x^{(i)}, y^{(i)}),\ \frac{\partial J}{\partial \theta_2}(\theta) = \frac{1}{m}\sum_{i=1}^{m} \frac{\partial loss}{\partial \theta_2}(\theta, x^{(i)}, y^{(i)}) \text{ etc}$$

* Pick a random sample of b points from the training data. Let N be the set of indices. Then use approx derivatives

$$DJ_{\theta_1}(\theta) = \frac{1}{b}\sum_{i\in N} \frac{\partial loss}{\partial \theta_1}(\theta, x^{(i)}, y^{(i)}),\ DJ_{\theta_2}(\theta) = \frac{1}{b}\sum_{i\in N} \frac{\partial loss}{\partial \theta_2}(\theta, x^{(i)}, y^{(i)}) \text{ etc}$$

* When $b = m$ and $N = \{1, 2, \ldots, m\}$ then we get back exact derivatives.

» Approximate Derivatives: Example

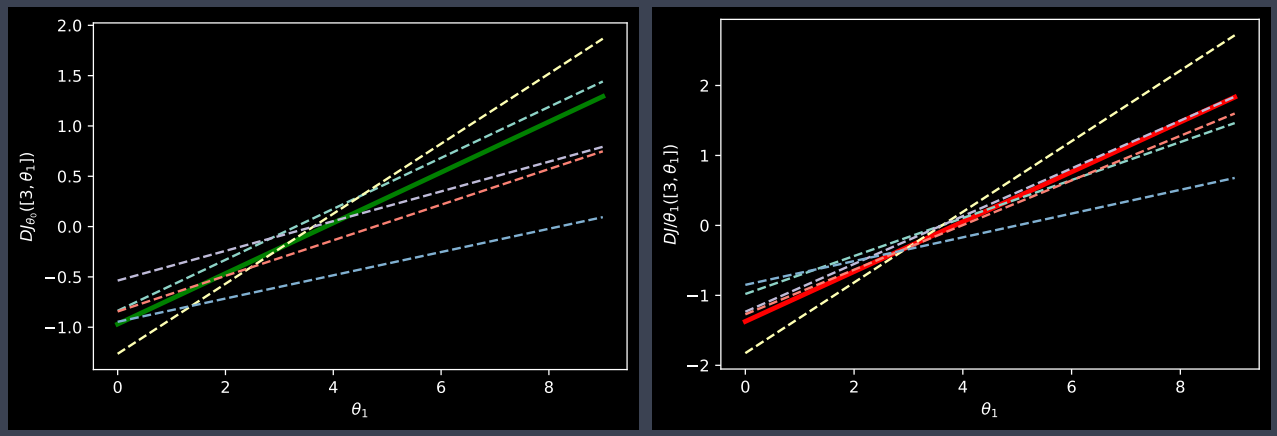
* Suppose we have $m = 100$ training data points $(x^{(i)}, y^{(i)})$, $i = 1, 2, \ldots, 100$. Linear regression:
  $loss(\theta, x^{(i)}, y^{(i)}) = 0.5(\theta^T x^{(i)} - y^{(i)})^2$, $\frac{\partial loss}{\partial \theta_k}(\theta, x^{(i)}, y^{(i)}) = (\theta^T x^{(i)} - y^{(i)}) x_k^{(i)}$
  $J(\theta) = \frac{1}{100} \sum_{i=1}^{100} loss(\theta, x^{(i)}, y^{(i)})$, $\frac{\partial J}{\partial \theta_k}(\theta) = \frac{1}{100} \sum_{i=1}^{100} \frac{\partial loss}{\partial \theta_k}(\theta, x^{(i)}, y^{(i)})$
* Sample $b = 5$points randomly from training data e.g. $N = \{76, 75, 40, 66, 18\}$, approx derivative:

$$DJ_{\theta_1}(\theta) = \frac{1}{5} \sum_{i \in N} \frac{\partial loss}{\partial \theta_1}(\theta, x^{(i)}, y^{(i)}) = \frac{1}{5} \sum_{i \in N} (\theta^T x^{(i)} - y^{(i)}) x_1^{(i)}$$

and so on for $\theta_2, \ldots, \theta_n$

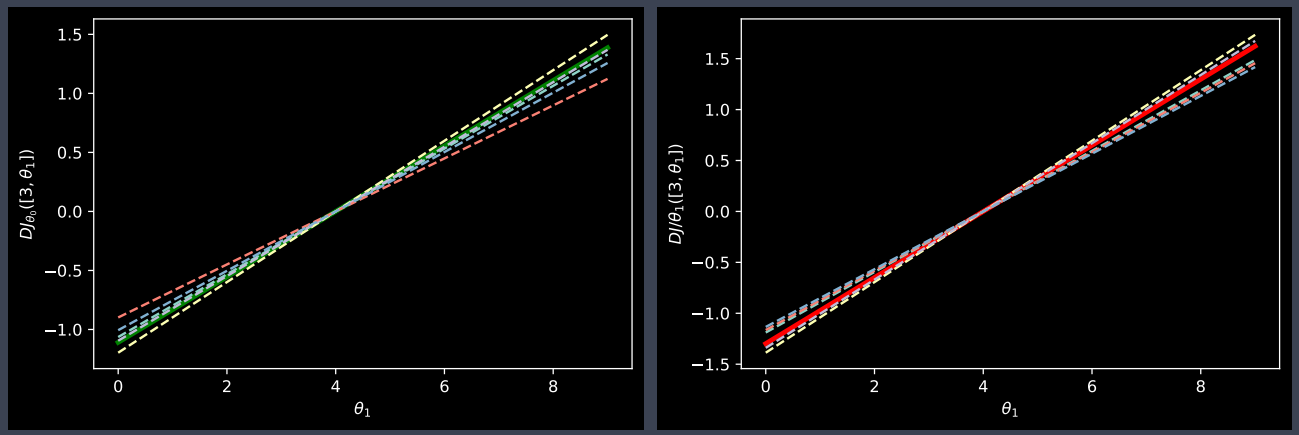
» Approximate Derivatives: Example

* Example: $f = x^2$, training data is 100 points with $x^{(i)}$ random and $y^{(i)} = (x^{(i)})^2 + \textit{noise}$.
* Draw 5 random training data points and calc approx derivative. Repeat 5 times (so get 5 different approximations to the derivative):



Solid lines indicate exact derivative

* Now use 50 random training data points to calc approx derivative:



Observe the approximate derivatives tend to be more accurate now.

» How to Sample?

- In above example we sampled 5 points with replacement from the 100 training data points. But this might mean that we don't use some of our training data, even after drawing repeated samples.
- Periodic sampling is more common:
  - Shuffle (i.e. randomly permute) training data
  - For first sample take points 1,2,...,5 from data
  - For second sample take points 6,7,...,10 from data
  - and so on
  - After doing this $n/5$ times we will have used all of our training data

» Mini-Batch Stochastic Gradient Descent (SGD)

* Modifying gradient descent to use approx derivatives and periodic sampling:

  $\theta = \theta 0,$ *batch_size* $= 5,$ *n* = #training data points

  for *k* in range(num_iters):

    shuffle training data

    for *i* in np.arange(0,*n*,*batch_size*):

      sample *N*=np.arange($i, i +$ *batch_size*)

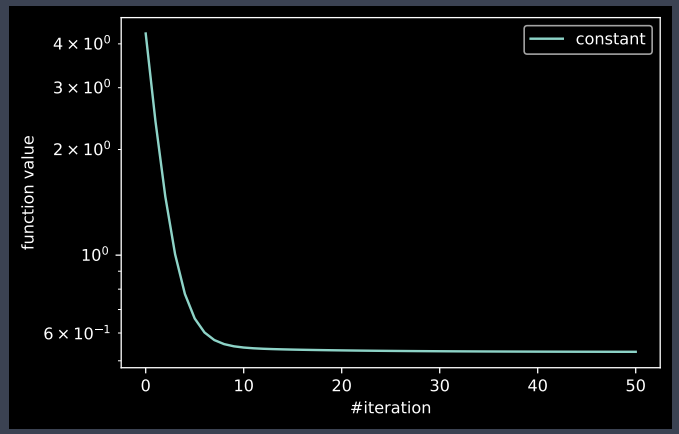
      calc approx derivative $DJ(\theta) = [DJ_{\theta_0}(\theta), DJ_{\theta_1}(\theta), \ldots, DJ_{\theta_n}(\theta)]$

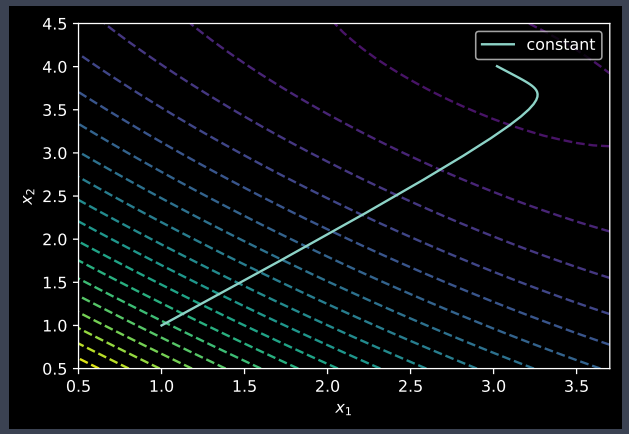
      $\theta = \theta - \alpha DJ(\theta)$

* Each run through the inner for-loop is called an *epoch* (corresponding to one run through the full training data).
* *Why do this? When #training data points n is v large, calculating approx derivative from small sample can be much faster than calculating exact derivative, yet still good enough to find downhill direction.*
* Mini-batch SGD is the standard approach with neural nets

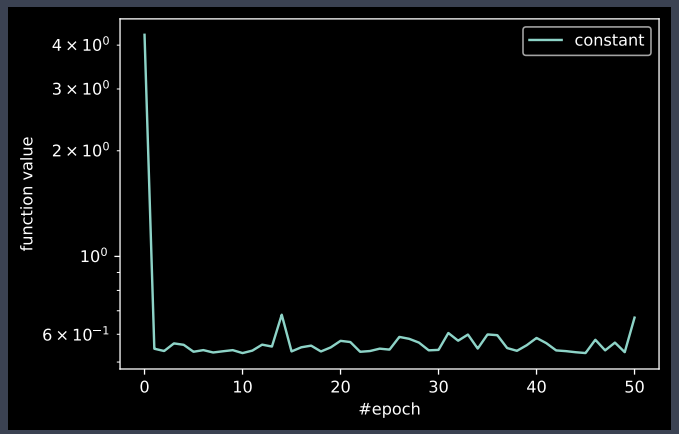
» Example

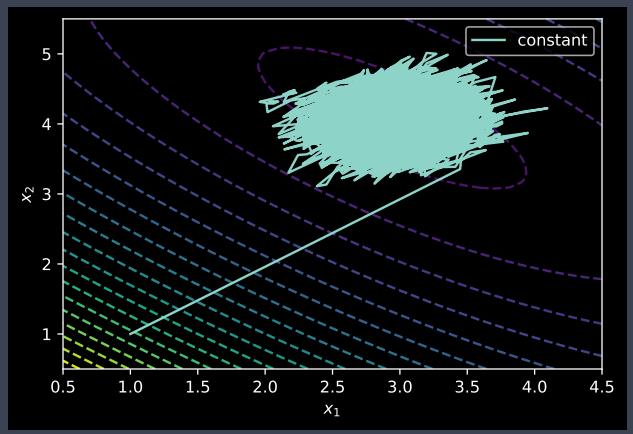
* Quadratic loss $m = 1000$ training data points, $y = \theta^T x + \textit{noise}$ with $\theta = [3, 4]$, starting point $x = [1, 1]$, constant $\alpha_0 = 0.5$





* Mini-batch SGD, batch size 5

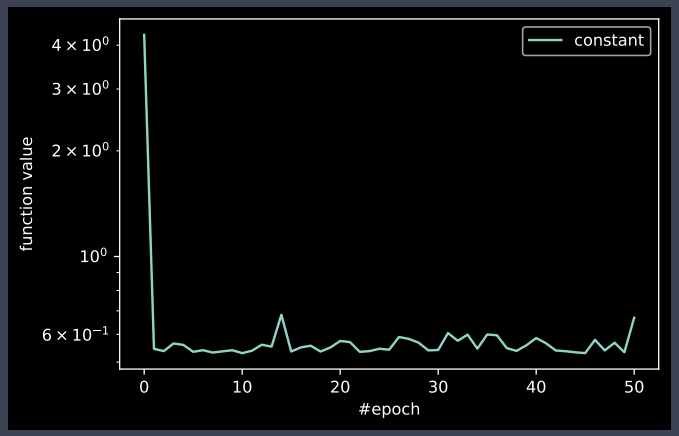


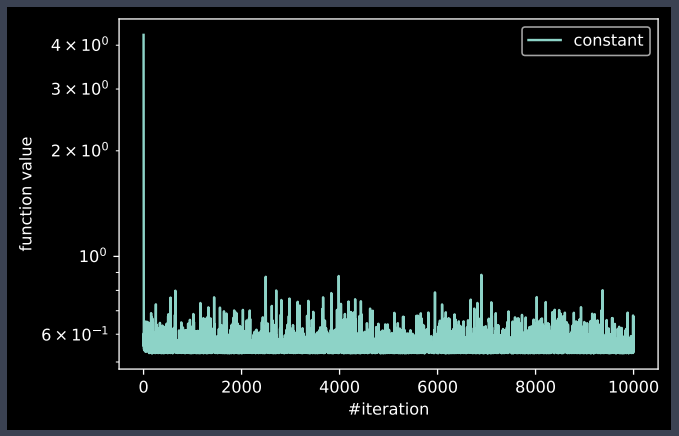


* For SGD one epoch is one run through training data $\rightarrow$ x has been updated $m/\textit{batch\_size}$ times. For GD one iteration is one update of x.
* With SGD get fast initial convergence, but when close to minimum the "noise" in the approx derivative causes x to "wander"

» Example

* Mini-batch SGD, batch size 5

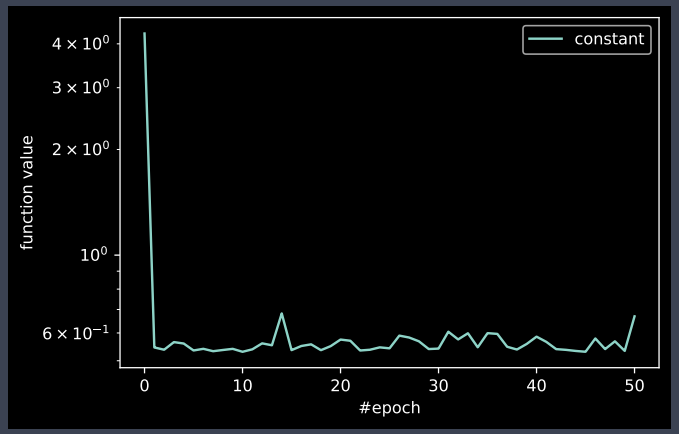


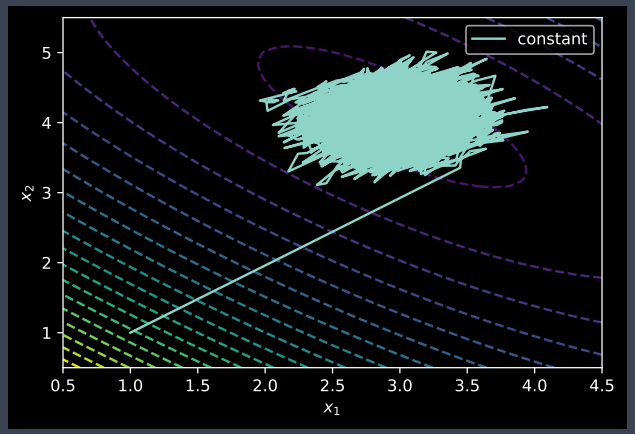


* Iteration here = an update to x, so one run of inner mini-batch loop
* Epoch = one run through all the mini-batches, so one run of outer loop.
* Epoch = $m/batch\_size = 1000/5 = 200$ iterations, so 50 epochs =10000 iterations

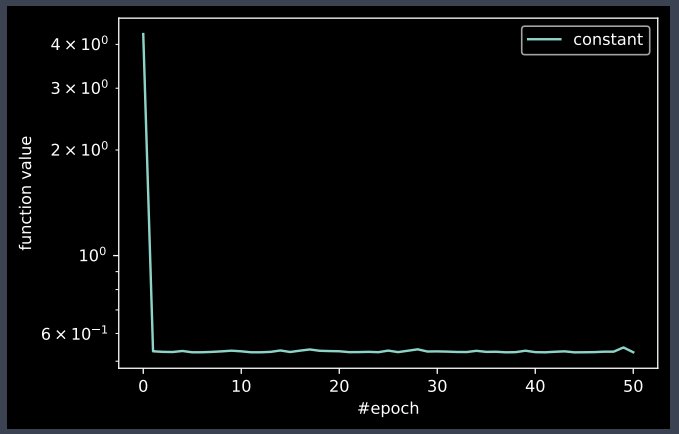
» Example

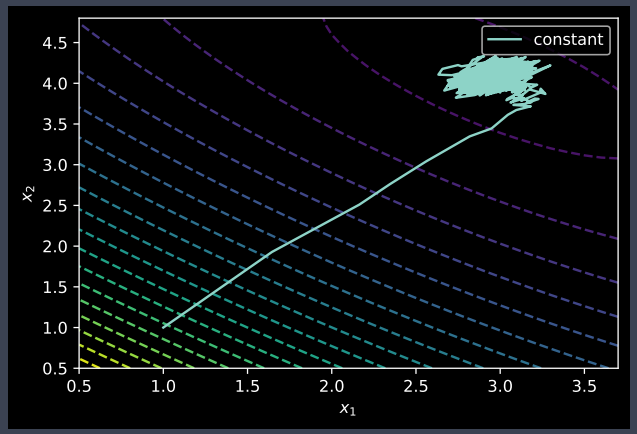
* Mini-batch SGD, batch size 5





* Mini-batch SGD, batch size 25

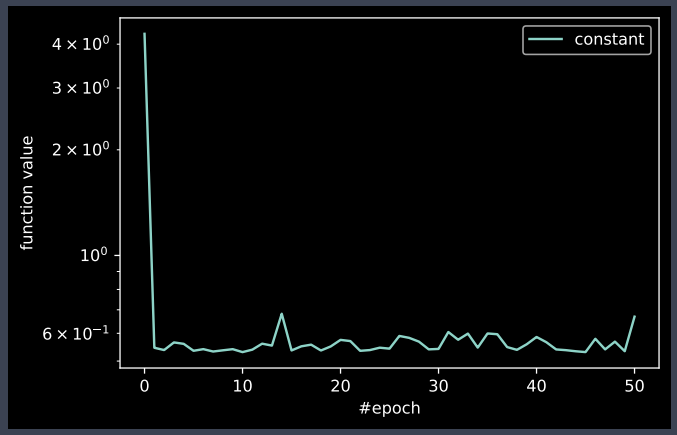


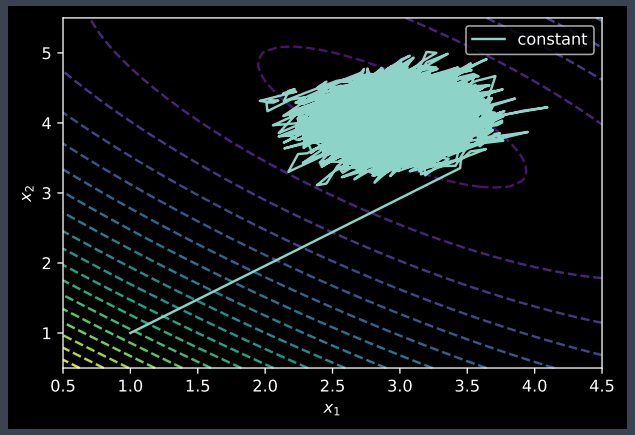


* Increasing batch size reduces the "noise" in the approx derivative and reduces wandering by x when close to minimum.
* Also slows fast initial convergence?

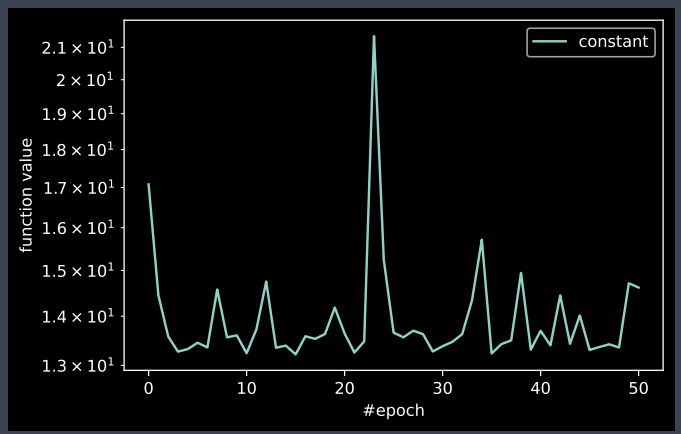
» Example

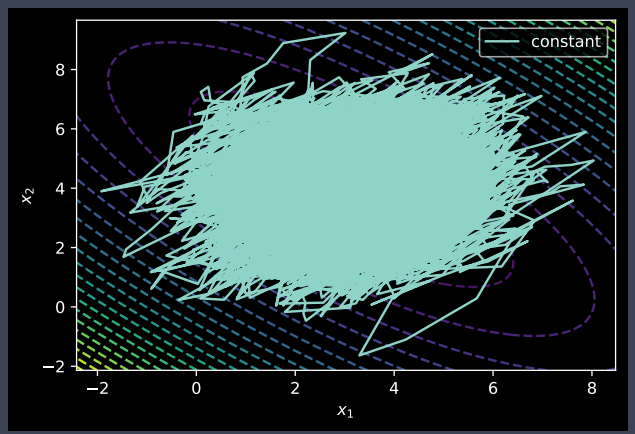
* Quadratic loss $m = 1000$ training data points, $y = \theta^T x + \textit{noise}$ with $\theta = [3, 4]$, starting point $x = [1, 1]$, constant $\alpha_0 = 0.5$
* Output y noise std deviation 1, mini-batch SGD, batch size 5





* Output y noise std deviation 5, mini-batch SGD, batch size 5

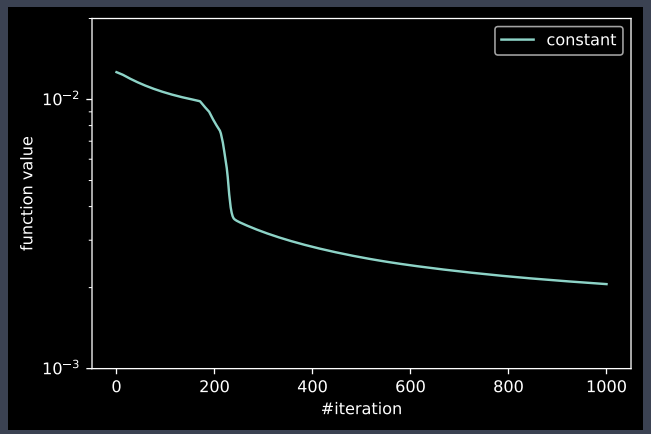


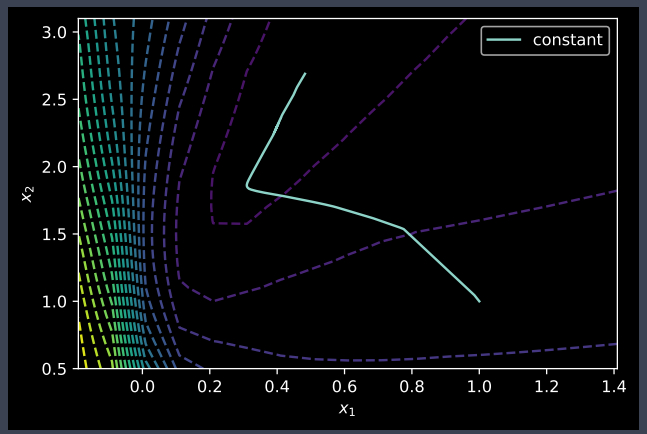


* More measurement noise causes mini-batch derivative estimate to get less accurate, x wanders a lot more

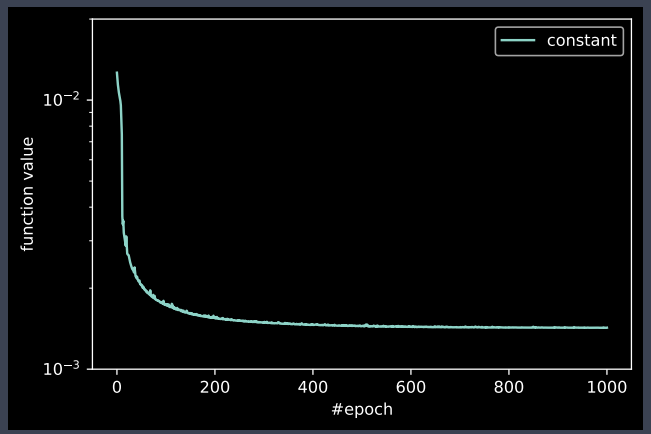
» Example

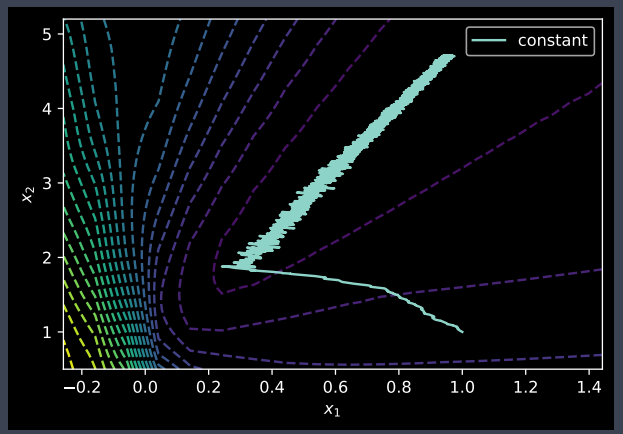
* Toy neural net $m = 100$ training data points, output y noise with std dev 0.05, starting point $x = [1, 1]$, constant $\alpha_0 = 0.75$





* Mini-batch SGD, batch size 5





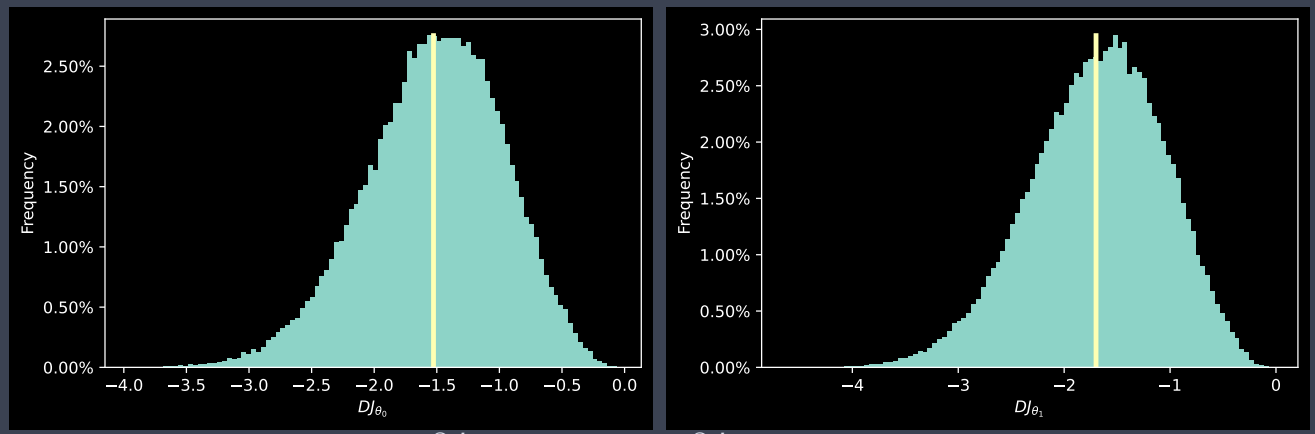
* Faster initial convergence with SGD

» Why Does Initial Convergence Seem Faster With SGD?

* Pick a random mini-batch sample from the training data. Let N be the indices. Then use approx derivatives:

$$DJ_{\theta_1}(\theta; N) = \sum_{i \in N} \frac{\partial loss}{\partial \theta_1}(\theta, x^{(i)}, y^{(i)}),\ DJ_{\theta_2}(\theta) = \sum_{i \in N} \frac{\partial loss}{\partial \theta_2}(\theta, x^{(i)}, y^{(i)}) \text{ etc}$$

* When $N = \{1, 2, \ldots, m\}$ then we get back exact derivatives.
* Suppose we repeately draw random samples, calc $DJ_{\theta_1}(\theta)$ and plot the values. E.g. Quadratic loss and $y = \theta^T x + noise$, $\theta = [3, 4]$:



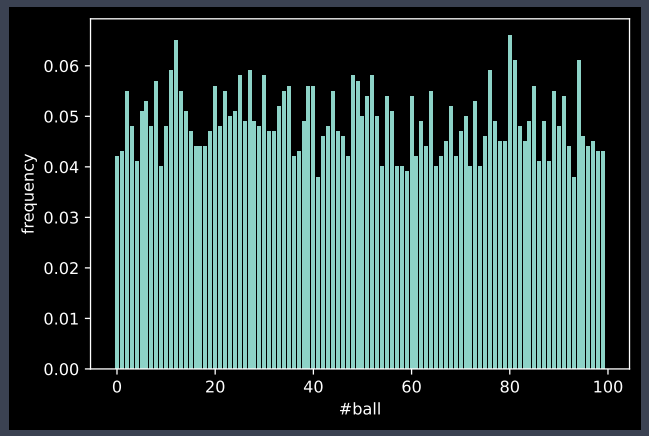
$$\frac{\partial J}{\partial \theta_0} = -1.526,\ \frac{\partial J}{\partial \theta_1} = -1.699$$

* The approximate derivatives DJ_{θ_i} take values around the exact derivatives $\frac{\partial J}{\partial \theta_i}$, $i = 0, 1$. *Why?*

» Why Does Initial Convergence Seem Faster With SGD?

Think about drawing balls from a bag:

* Suppose I have a bag with m different balls in it.
* I reach into the bag to draw out a ball, each ball has probability $1/m$ of being picked.
* After picking a ball, I put it back in the bag i.e. *sample with replacement*
* Repeat this b times, so selecting a batch of b balls.
* Each ball in the bag will on average appear b/m times in the batch, e.g. $m = 100$, $b = 5$ and repeat experiment $M = 1000$ times:




```
m=100; b=5; M=1000
count=np.zeros(m)
for k in range(M):
    batch=[]
    for i in range(b):
        batch.append(np.random.randint(0,m))
    count[batch] = count[batch]+1
plt.bar(range(m),count/M)
```

» Why Does Initial Convergence Seem Faster With SGD?

* Pick a random mini-batch of b samples from the training data, repeat M times and let N_k be the indices of the k'th sample. The k'th approx derivative is:

$$DJ_{\theta_1}(\theta; N_k) = \frac{1}{b} \sum_{i \in N_k} \frac{\partial loss}{\partial \theta_1}(\theta, x^{(i)}, y^{(i)})$$

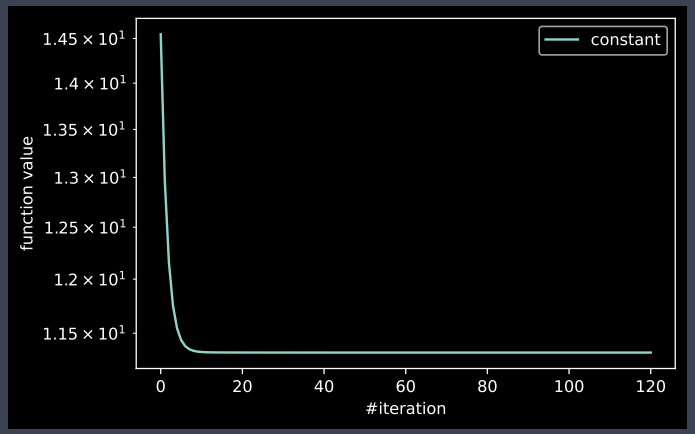
* There are m training data points. Each point in the training data is selected to be in sample N_k with probability b/m (cf bag with m balls from which we draw batches of size b).
* Over M runs training point i will on average be selected Mb/m times i.e.

$$\frac{1}{M} \sum_{k=1}^{M} \frac{1}{b} \sum_{i \in N_k} \frac{\partial loss}{\partial \theta_1}(\theta, x^{(i)}, y^{(i)}) \approx \frac{Mb/m}{Mb} \sum_{i=1}^{m} \frac{\partial loss}{\partial \theta_1}(\theta, x^{(i)}, y^{(i)}) = \frac{\partial J}{\partial \theta_1}(\theta)$$

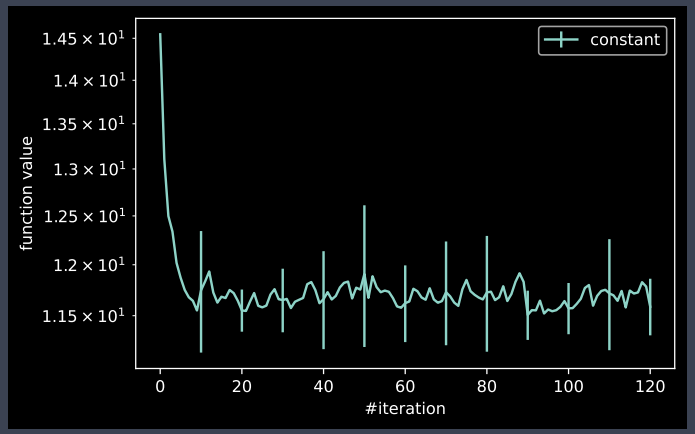
* *So the way that we sample mini-batches ensures that the empirical mean of the approx derivative equals to the exact derivative.*
* Can think of $DJ_{\theta_1}(\theta; N_k) = \frac{\partial J}{\partial \theta_1}(\theta) + noise_k$, with $E[noise_k] = 0$
* i.e. $\frac{1}{M} \sum_{k=1}^{M} DJ_{\theta_1}(\theta; N_k) = \frac{\partial J}{\partial \theta_1}(\theta) + \frac{1}{M} \sum_{k=1}^{M} noise_k \to \frac{\partial J}{\partial \theta_1}(\theta)$ as $M \to \infty$

» Why Does Initial Convergence Seem Faster With SGD?

* Quadratic loss $m = 100$ training data points, $y = \theta^T x + \textit{noise}$ with $\theta = [3, 4]$, starting point $x = [1, 1]$, constant $\alpha_0 = 0.5$



Gradient descent

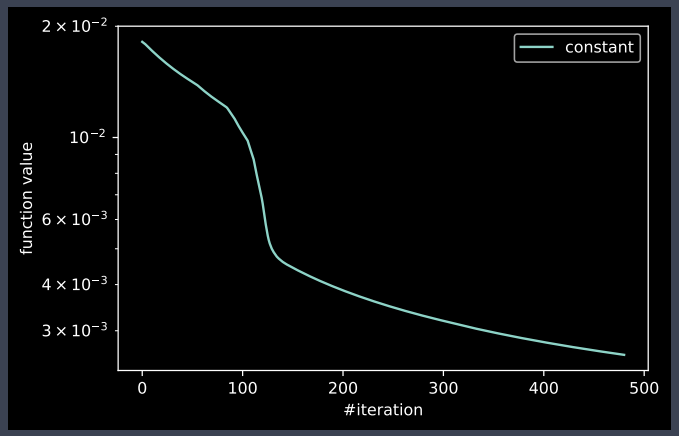


Mini-batch SGD, batch size 5. Repeat $M = 25$ times

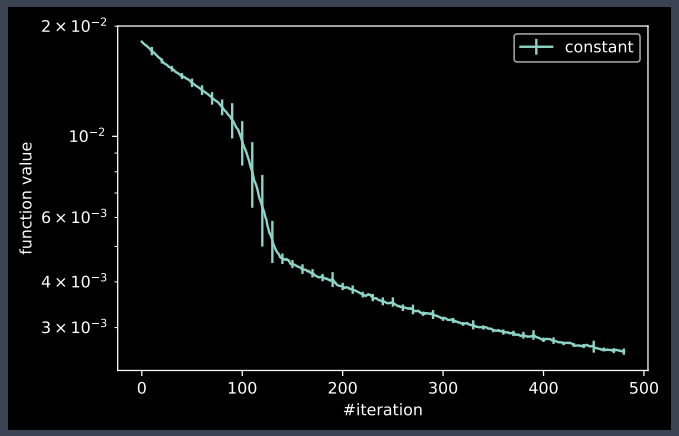
* SGD plot: solid line is emprical mean over the M runs, error bars indicate one standard deviation, x-axis is mini-batch inner loop iterations, *not epochs*.
* See that on average the convergence rate of SGD matches that of gradient descent when we compare iterations (rather than epochs)
* *One iteration of SGD is much cheaper than one iteration of gradient descent*

» Why Does Initial Convergence Seem Faster With SGD?

* Toy neural net $m = 100$ training data points, output y noise with std dev 0.05, starting point $x = [1, 1]$, constant $\alpha_0 = 0.75$



Gradient descent



Mini-batch SGD, batch size 5. Repeat $M = 25$ times

» Sampling Strategy

* In above analysis we selected each training point *uniformly at random with replacement* and treat mini-batches *independently*.
  * Uniformly at random = every training point equally likely to be picked for inclusion in a mini-batch.
  * With replacement = we put ball back in bag after picking it, so there's a chance the same ball will be picked again i.e. a mini-batch may contain the same training point multiple times
  * Treat mini-batches independently = we repeat this process independently for each mini-batch, so the same training data point can also appear in two consecutive mini-batches
  * E.g. with $m = 10$ data points and mini-batch size 5 we might choose mini-batches:

$$\{5, 3, 5, 1, 2\}, \{1, 4, 6, 2, 5\}, \{3, 2, 6, 4, 4\}$$

» Sampling Strategy

- Alternative: selected each training point *uniformly at random without replacement* and treat mini-batches *independently*. .
  - Uniformly at random = every training point equally likely to be picked for inclusion in a mini-batch.
  - Without replacement = we *don't* put ball back in bag after picking it, so a training point can only appear once in a mini-batch
  - When number of training data points is large (as it usually is when using SGD) then with/without replacement strategies are much the same (the chance of choosing the same training point multiple times in a mini-batch is really small)
  - Treat mini-batches independently = we repeat this independently for each mini-batch, so the same training data point can also appear in two consecutive mini-batches even though the same point cannot appear twice within the same mini-batch
  - E.g. with $m = 10$ data points and mini-batch size 5 we might choose mini-batches:

$$\{5, 3, 1, 2, 4\}, \{1, 4, 6, 2, 5\}, \{3, 2, 6, 1, 4\}$$

» Sampling Strategy

* Alternative (more common): select each training point once over an epoch, but *in random order*. E.g. its what this code does:

$\theta = \theta 0,\ batch\_size = 5,\ n =$ #training data points
for *k* in range(num_iters):
    shuffle training data
    for *i* in np.arange(0,*n*,*batch_size*):
        sample *N*=np.arange(*i*, $i +$ *batch_size*)
        calc approx derivative $DJ(\theta) = [DJ_{\theta_0}(\theta), DJ_{\theta_1}(\theta), \ldots, DJ_{\theta_n}(\theta)]$
        $\theta = \theta - \alpha DJ(\theta)$

* At iteration 1 of inner loop the mini-batch $N_1 = \{1, 2, \ldots, batch\_size\}$.
* Suppose we re-run above code many times. Due to the shuffling, the training points in mini-batch N_1 are selected uniformly at random without replacement.
* But the same training data point cannot appear in two consecutive mini-batches, so this shuffling sampling strategy is not quite the same as previous sampling without replacement strategy
* E.g. with $m = 10$ data points and mini-batch size 5 we might choose mini-batches:

$$\{5, 3, 1, 2, 4\}, \{8, 10, 6, 7, 9\}$$

* Hard to analyse, but in practice behaves much the same as the "sample uniformly at random with replacement and treat mini-batches independently" strategy.

» Sampling Strategy

* To be avoided: select each training point once over an epoch, but in *fixed order*. E.g. its what this code does:

$\theta = \theta 0,$ *batch_size* $= 5$, $n =$ #training data points
for *k* in range(num_iters):
~~shuffle training data~~
for *i* in np.arange(0,*n*,*batch_size*):
sample *N*=np.arange(*i*, *i* + *batch_size*)
calc approx derivative $DJ(\theta) = [DJ_{\theta_0}(\theta), DJ_{\theta_1}(\theta), \ldots, DJ_{\theta_n}(\theta)]$
$\theta = \theta - \alpha DJ(\theta)$

* Note the lack of a shuffle at the start of each run of the inner loop.
* Suppose our training data was ordered so that all the points of one type (e.g. all the examples with label +1) come first, then all points of a second type come next (e.g. all the examples with label -1) and so on.