Training Neural Networks: Optimization

Intro to Deep Learning, Fall 2022

Recap

- Neural networks are universal approximators
- We must *train* them to approximate any function
- Networks are trained to minimize total "error" on a training set
  - We do so through empirical risk minimization
- We use variants of gradient descent to do so
  - Gradients are computed through backpropagation

Recap

- Vanilla gradient descent may be too slow or unstable

- Better convergence can be obtained through
  - Second order methods that normalize the variation across dimensions
  - Adaptive or decaying learning rates that can improve convergence
  - Methods like Rprop that decouple the dimensions can improve convergence
  - Momentum methods which emphasize directions of steady improvement and deemphasize unstable directions

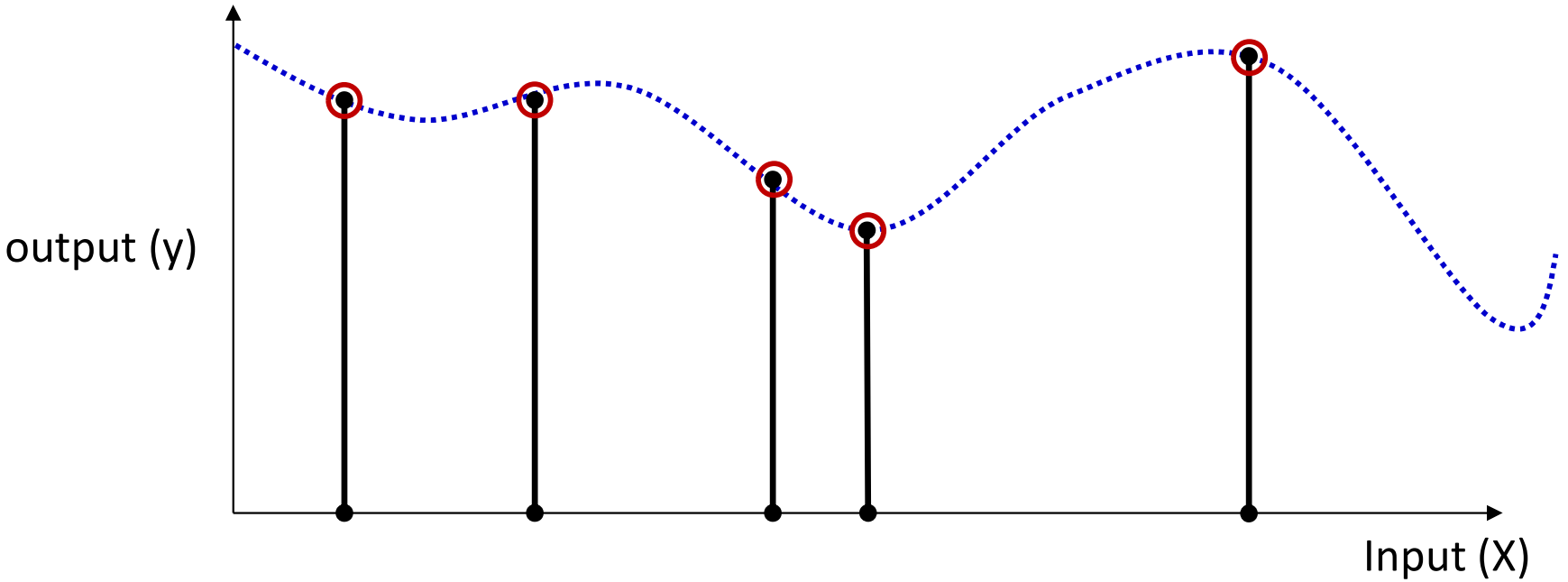
Moving on…

- Incremental updates
- Revisiting “trend” algorithms
- Generalization
- Tricks of the trade
  - Divergences..
  - Activations
  - Normalizations

Moving on: Topics for the day

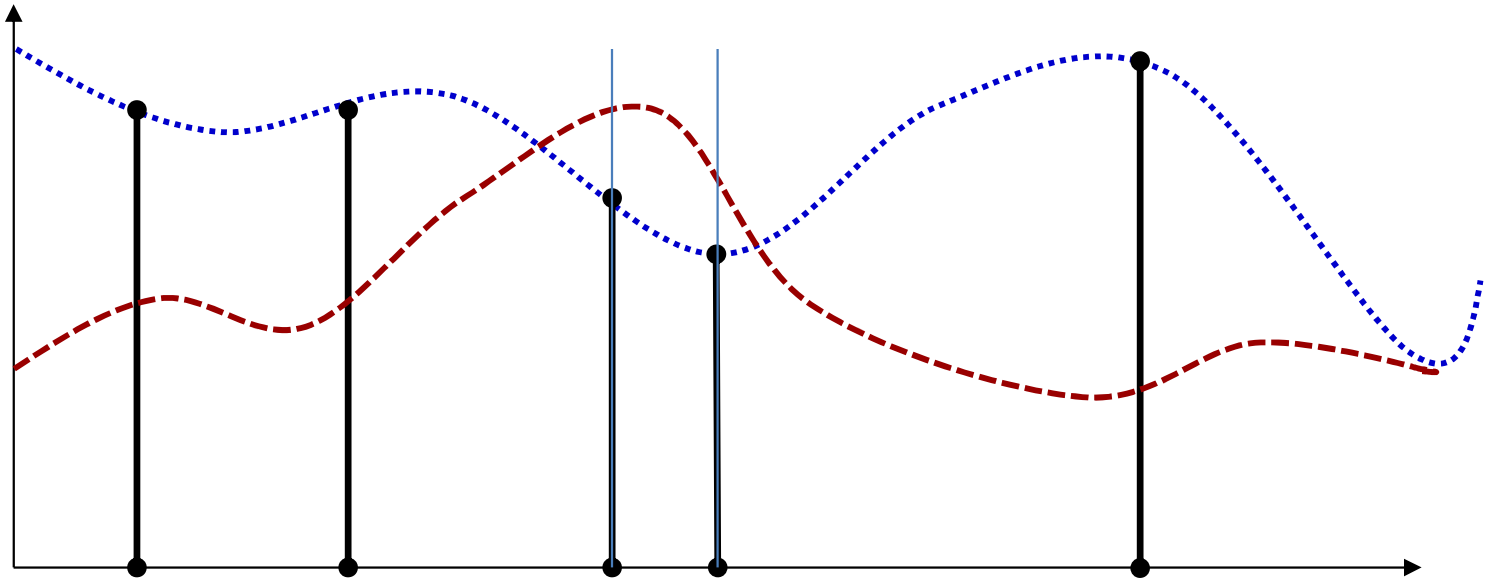
- Incremental updates
- Revisiting “trend” algorithms
- Generalization
- Tricks of the trade
  - Divergences..
  - Activations
  - Normalizations

The training formulation



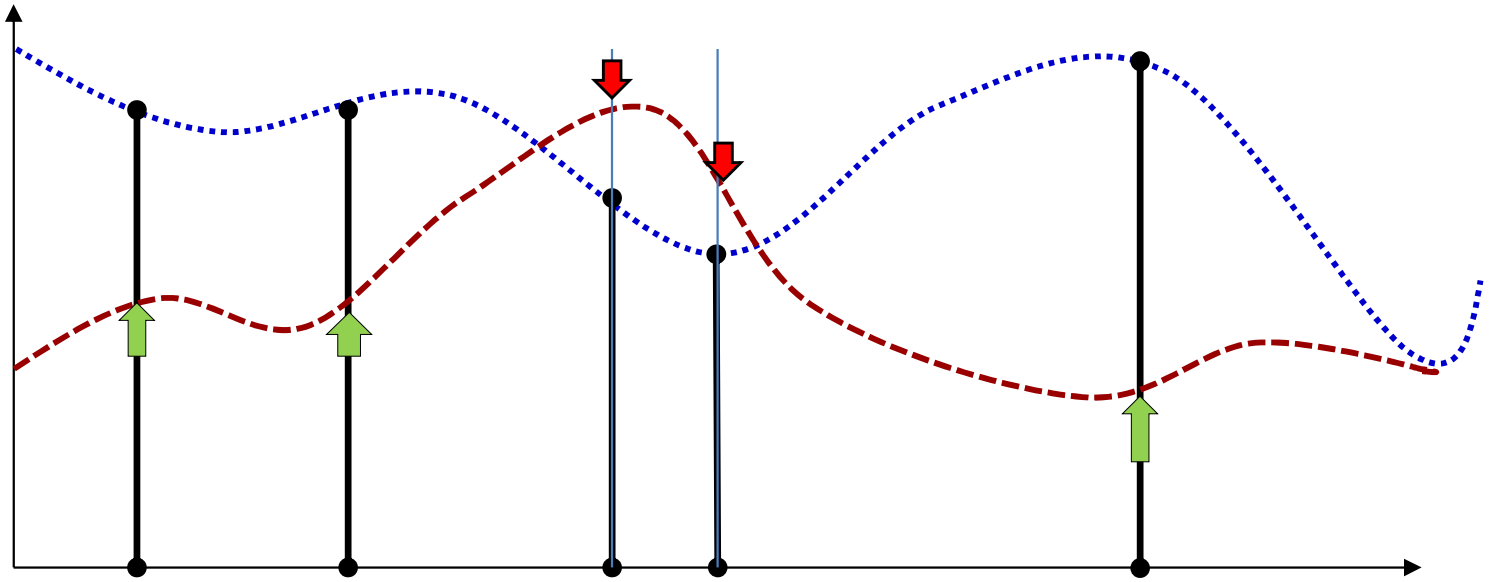
- Given input output pairs at a number of locations, estimate the entire function

Gradient descent



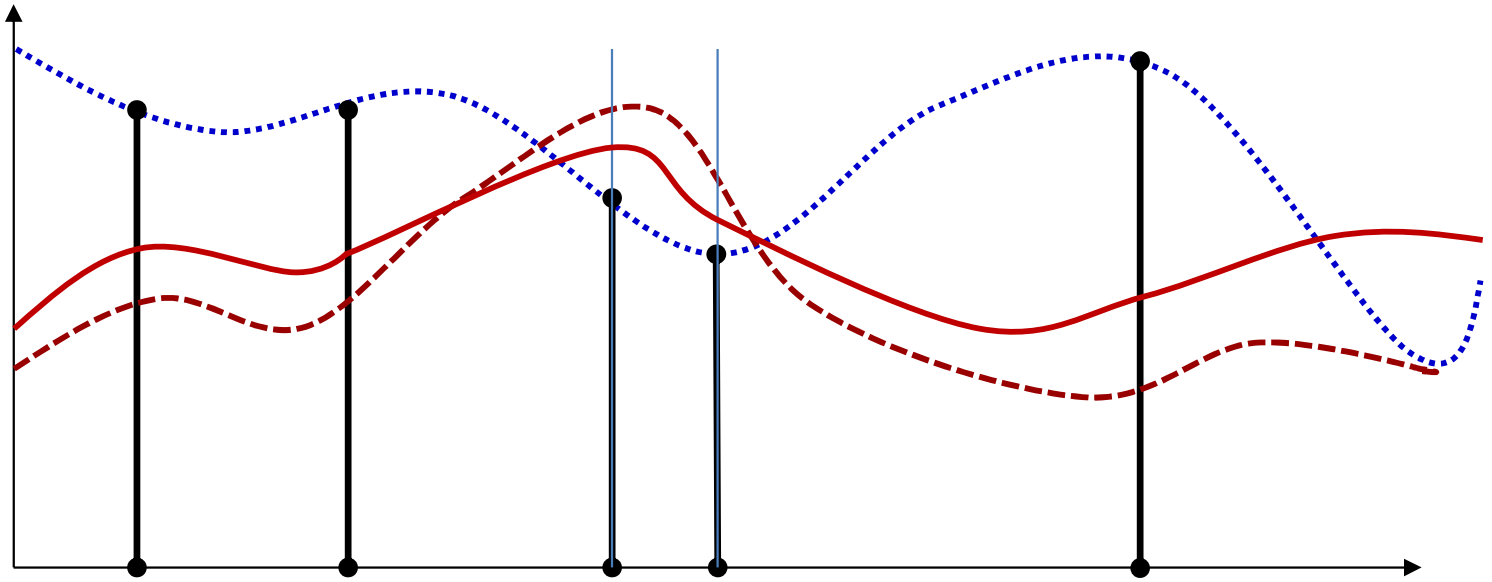
- Start with an initial function

Gradient descent



- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



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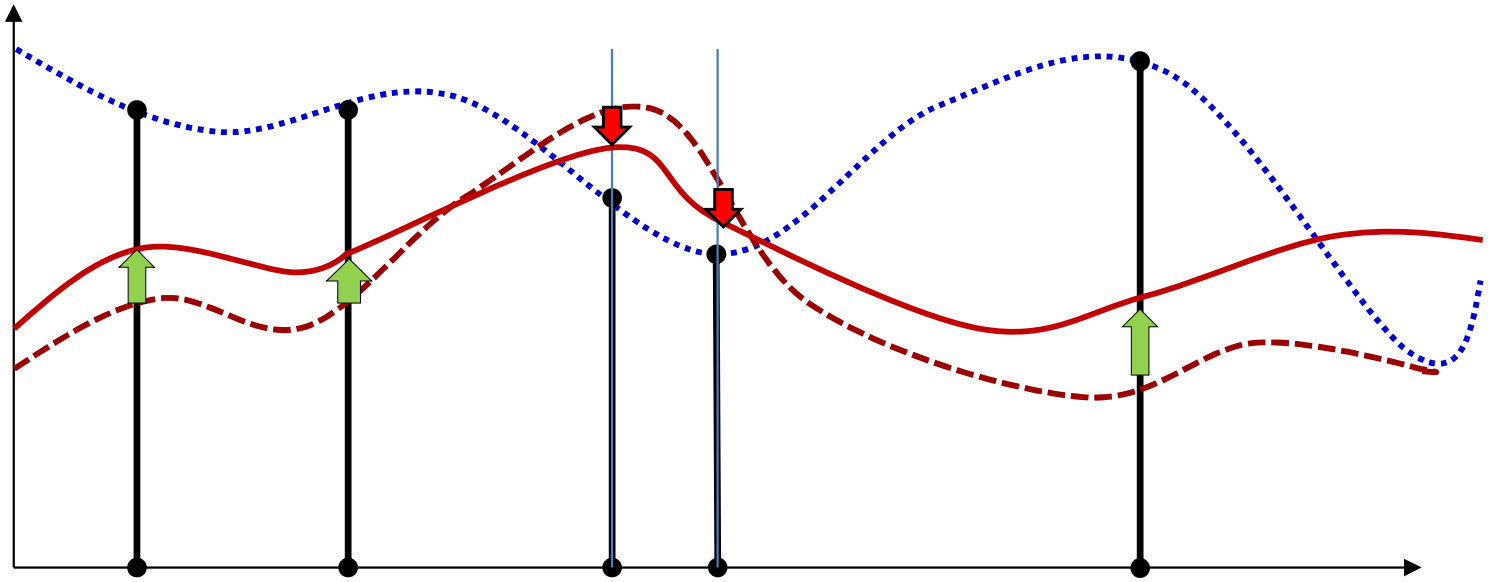

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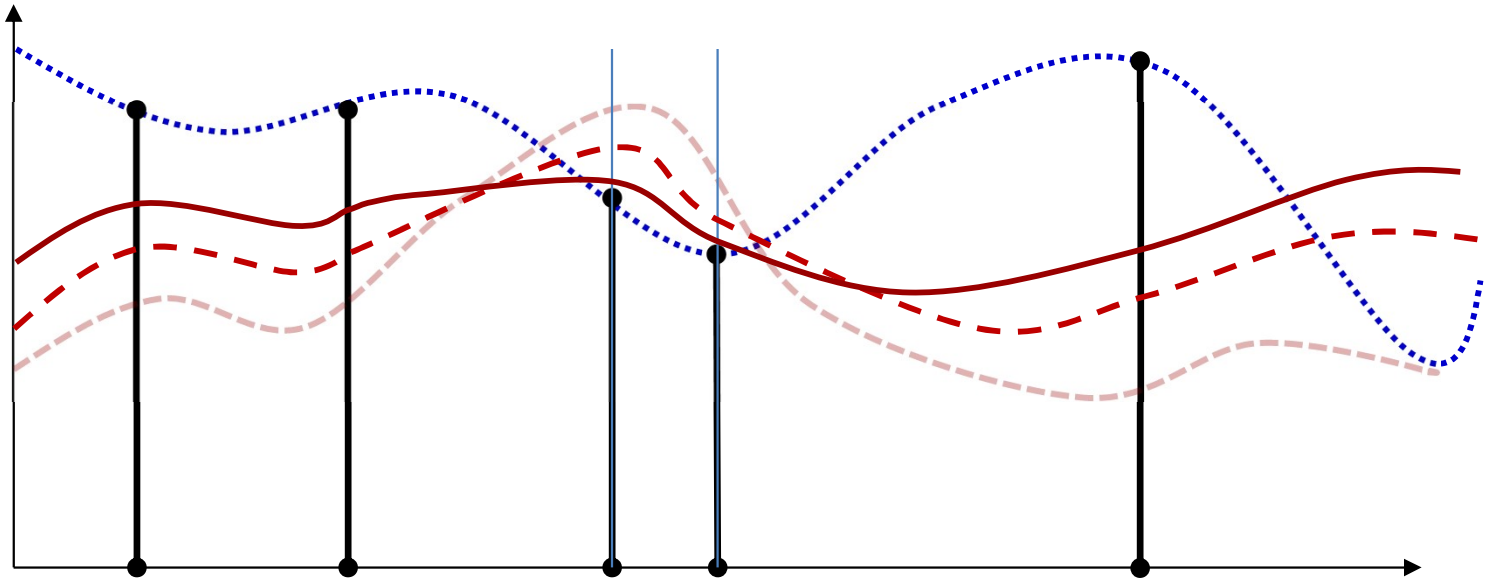

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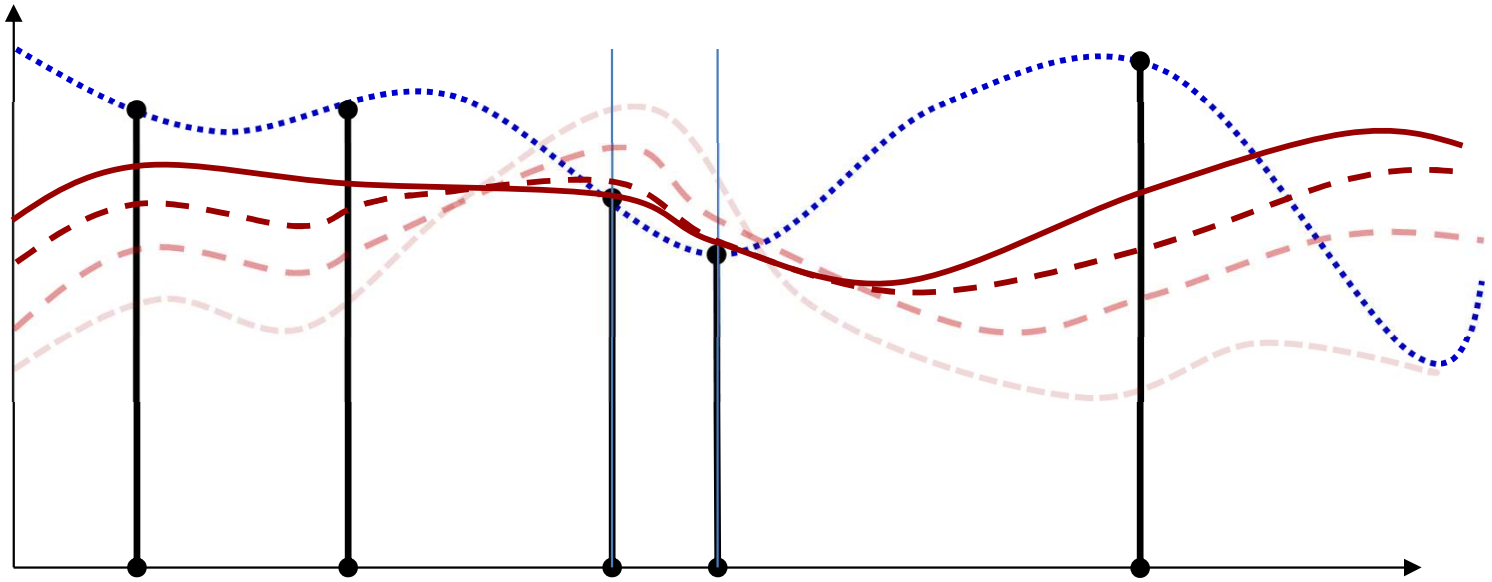

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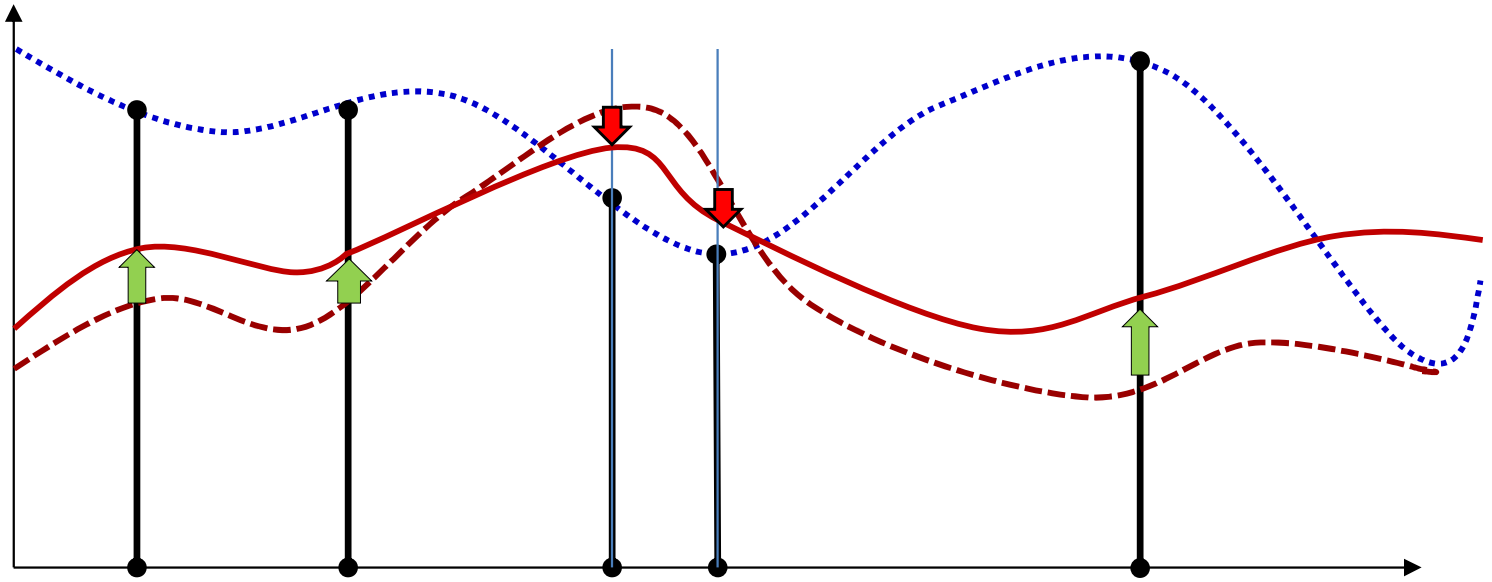
Effect of number of samples



- Problem with conventional gradient descent: we try to simultaneously adjust the function at *all* training points
  - We must process *all* training points before making a single adjustment
  - **"Batch"** update

Poll 1

PIAZZA @528

Select all that are true

- The actual loss function we try to minimize requires batch updates
- Batch updates minimize the total loss over the entire training data
- Batch updates optimize the actual loss function
- Batch updates require processing the entire training data before we perform a single update

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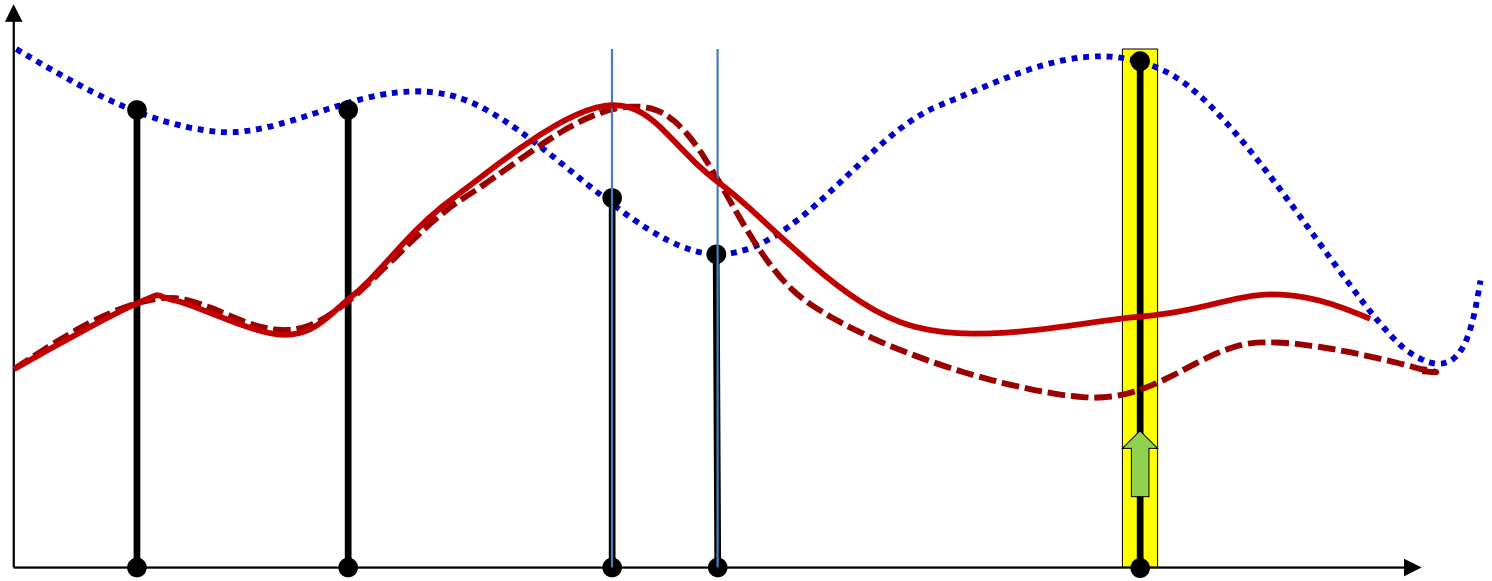
Alternative: Incremental update



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  - Keep adjustments small

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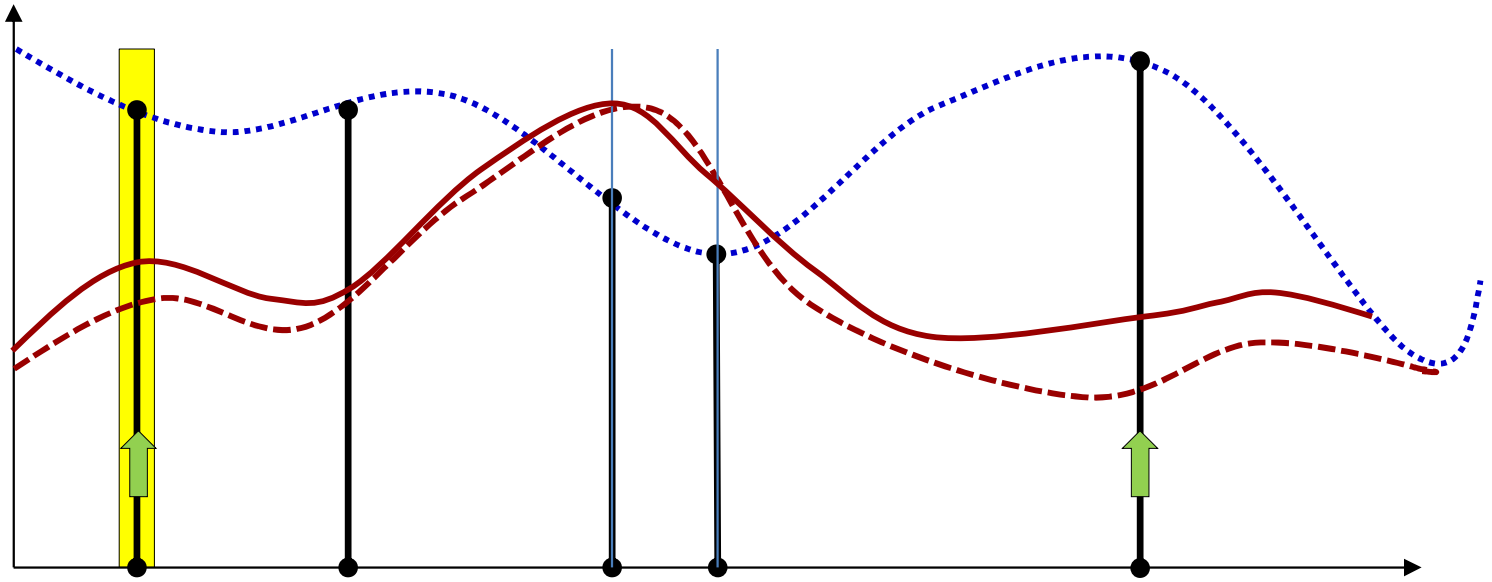

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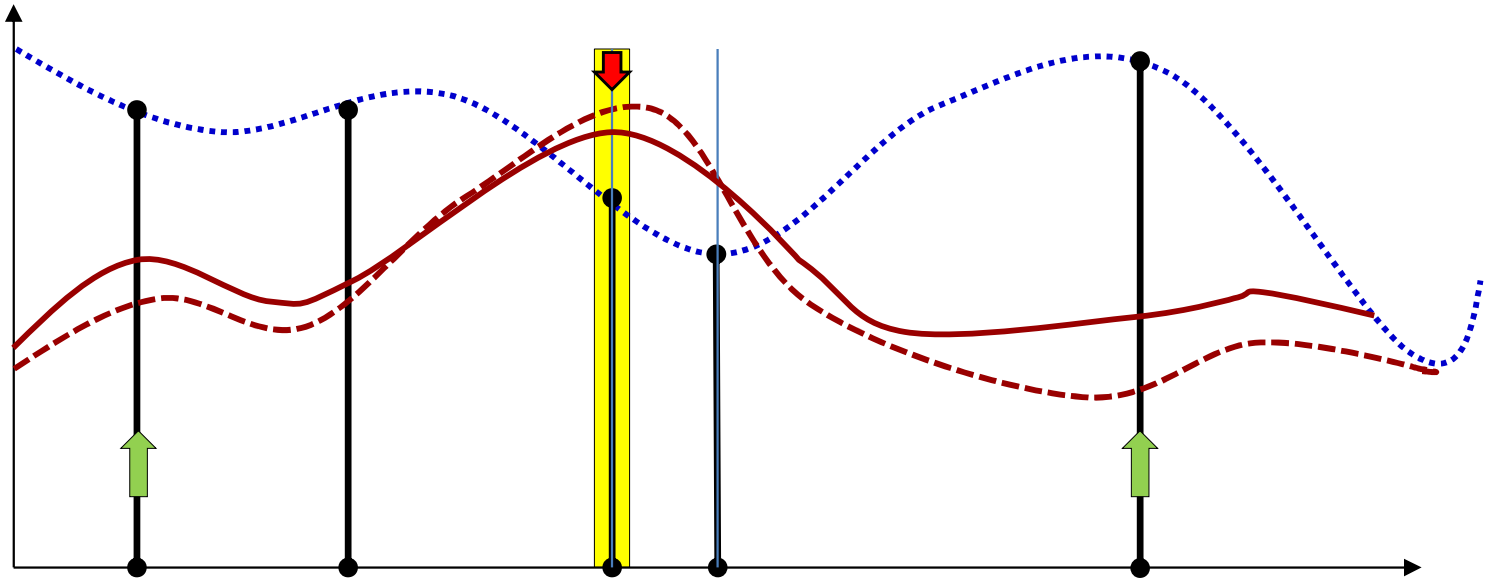

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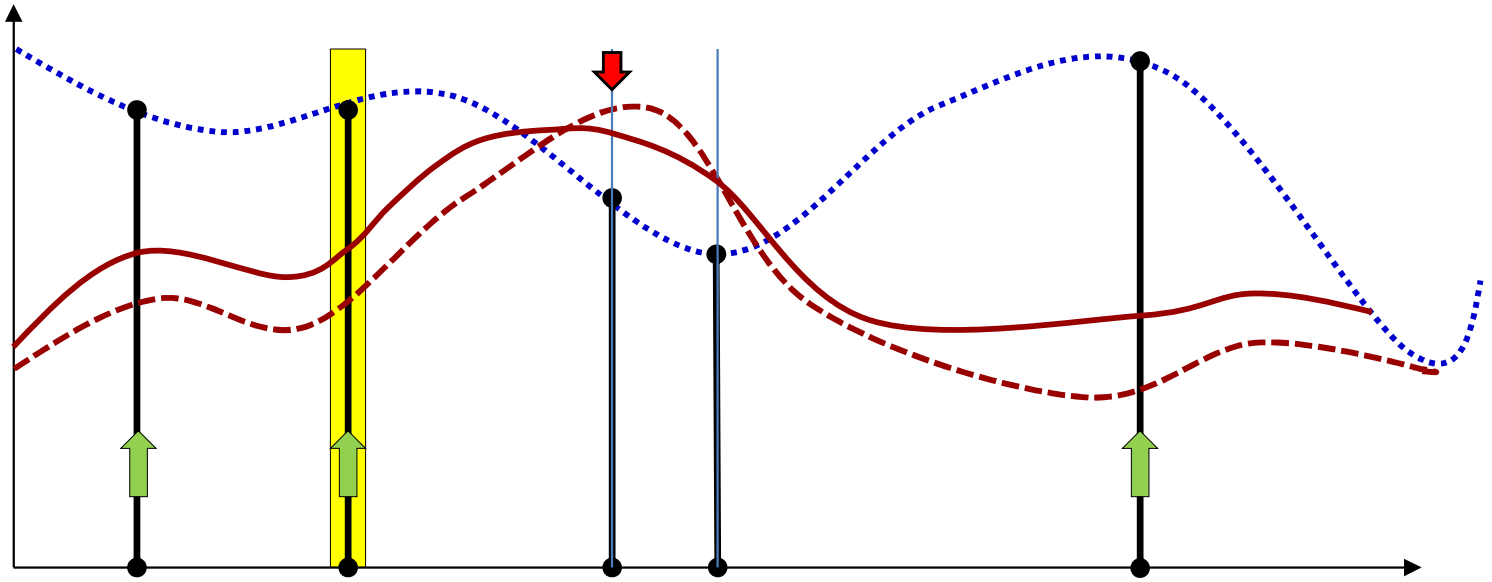

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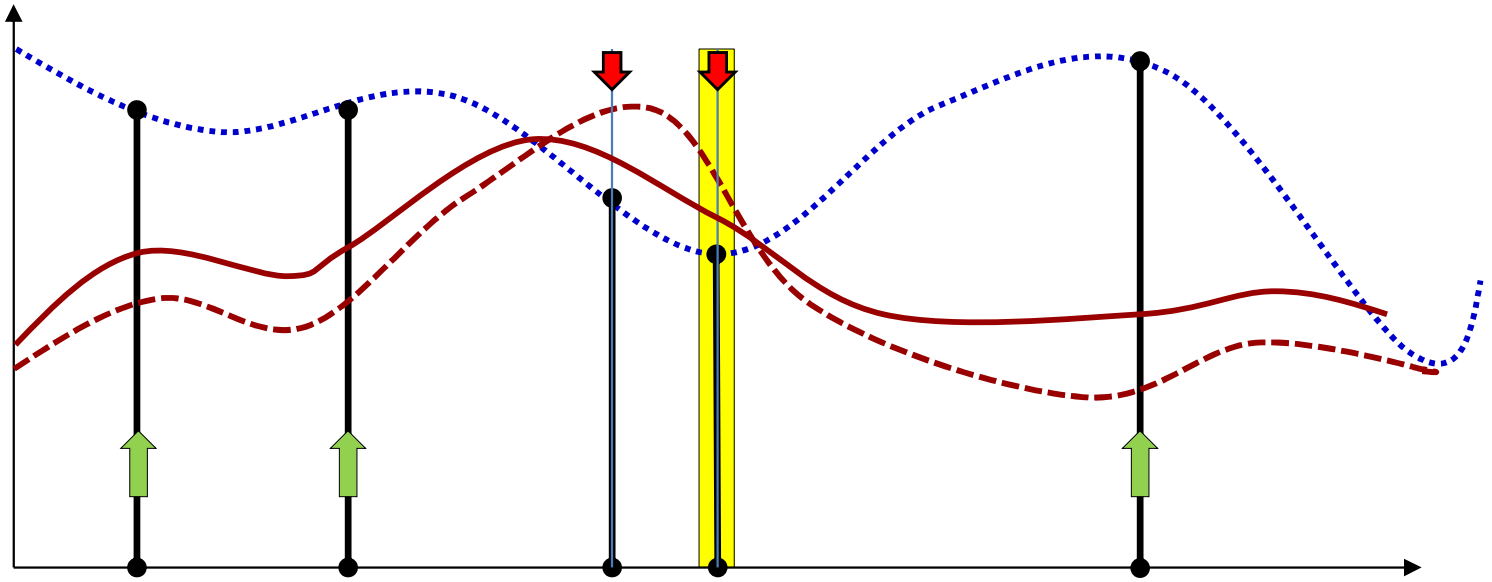

- Alternative: adjust the function at one training point at a time
  - Keep adjustments small
  - Eventually, when we have processed all the training points, we will have adjusted the entire function
    - With *greater* overall adjustment than we would if we made a single "Batch" update

Incremental Update

- Given $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- Initialize all weights $W_1, W_2, \ldots, W_K$
- Do:
  - For all $t = 1:T$
    - For every layer k:
      - Compute $\nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})$
      - Update

$$W_k = W_k - \eta \nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})^T$$

- Until $Loss$ has converged

Incremental Updates

- The iterations can make multiple passes over the data
- A single pass through the entire training data is called an “epoch”
  - An epoch over a training set with T samples results in T updates of parameters

Incremental Update

- Given $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- Initialize all weights $W_1, W_2, \ldots, W_K$
- Do: ← Over multiple epochs
  - For all $t = 1:T$ ← One epoch
    - For every layer k:
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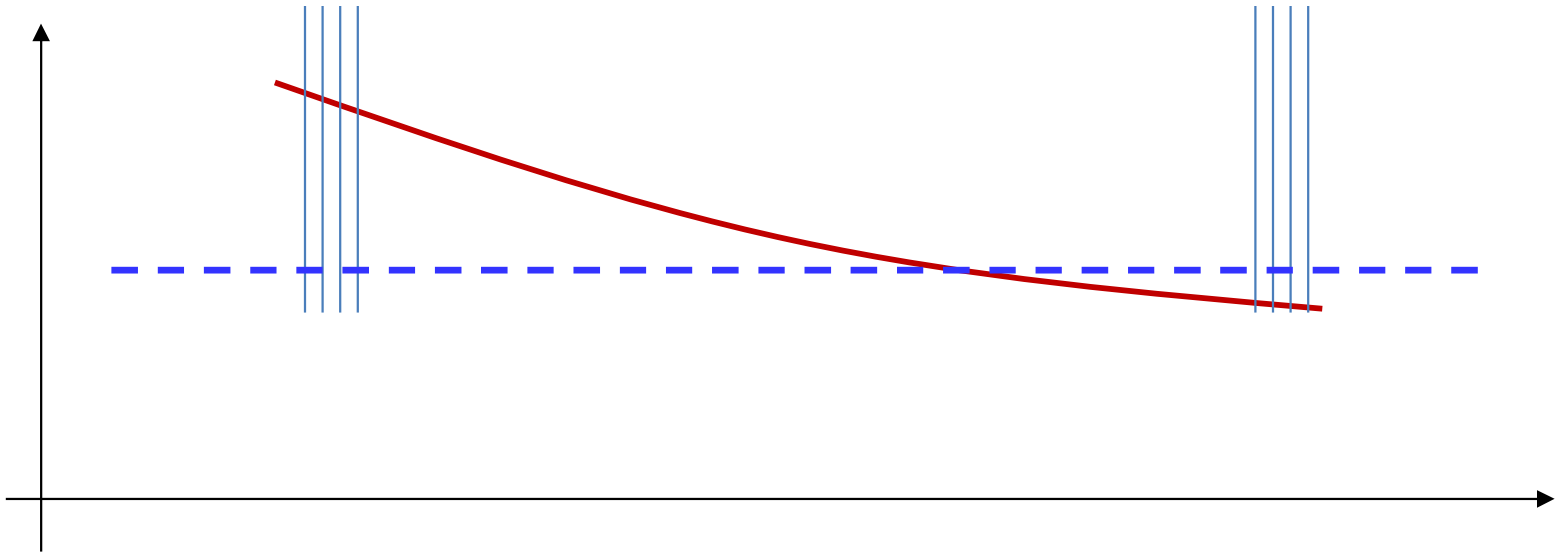
        $W_k = W_k - \eta \nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})^T$ ← One update
- Until $Loss$ has converged

Caveats: order of presentation



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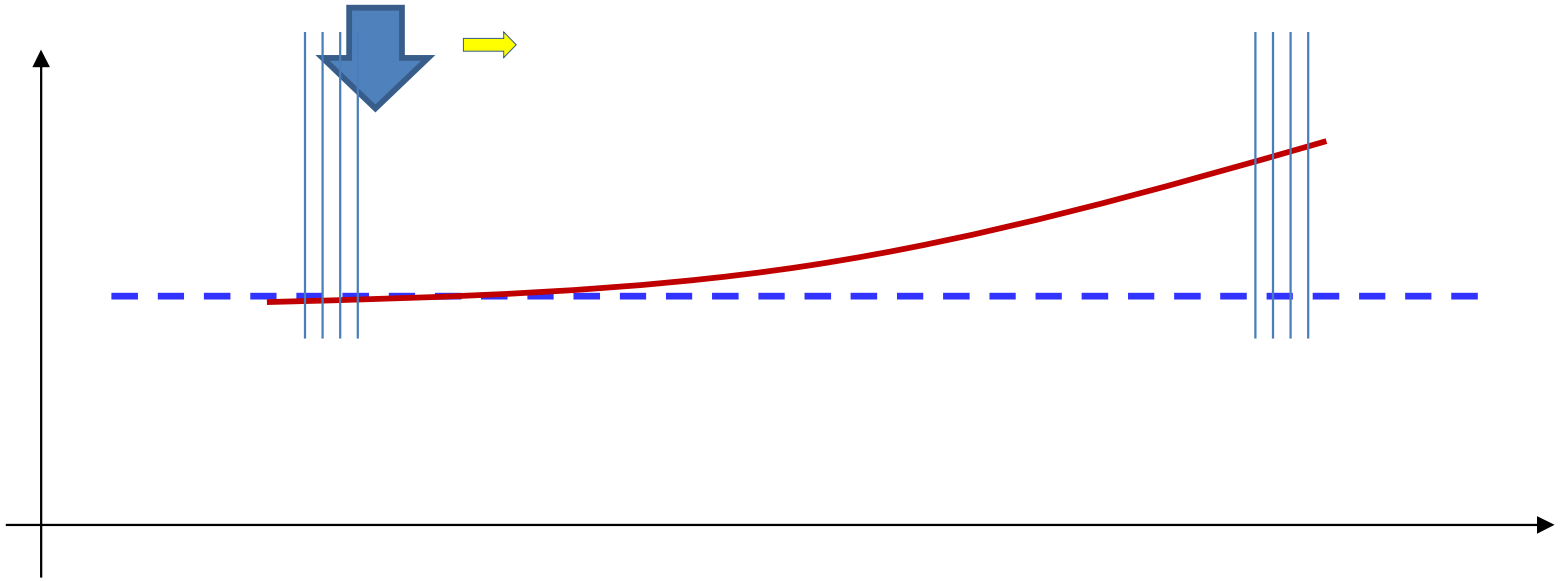

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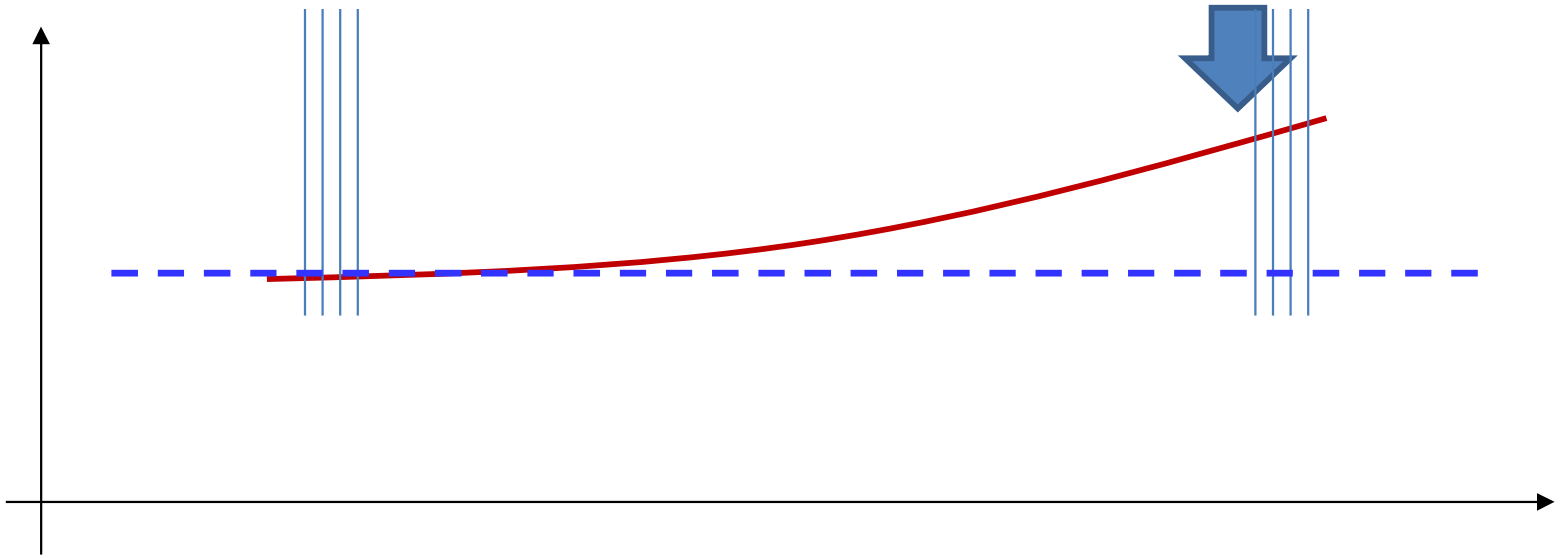

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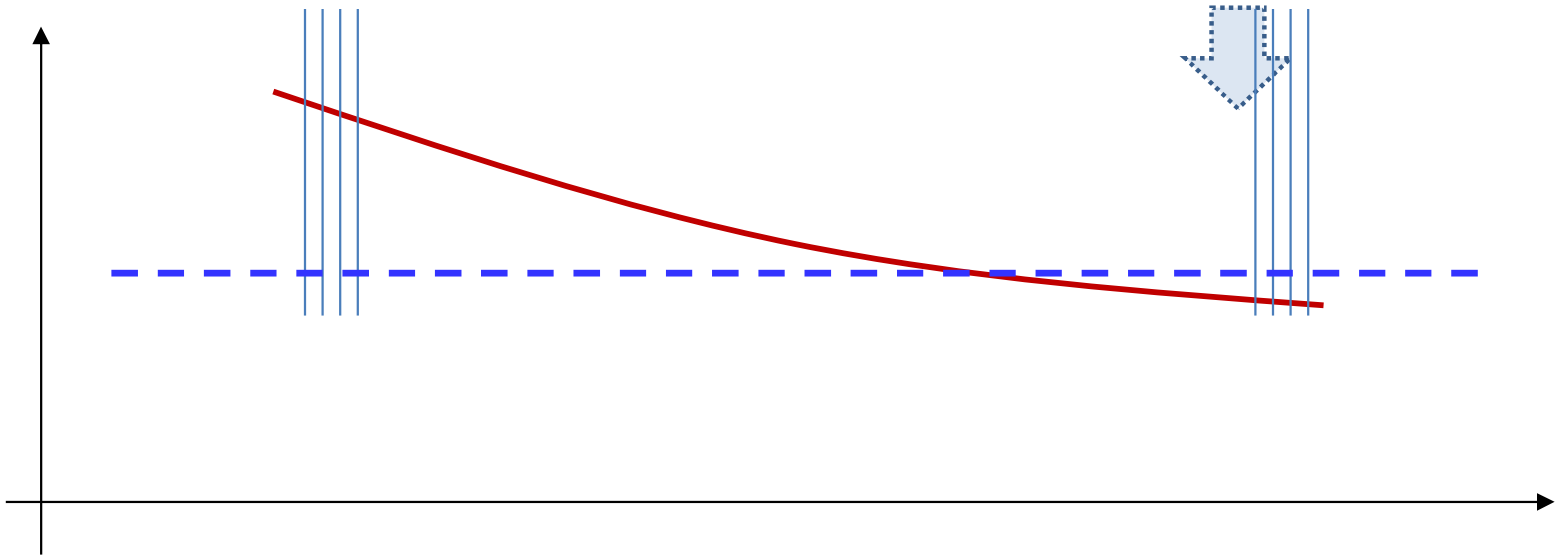

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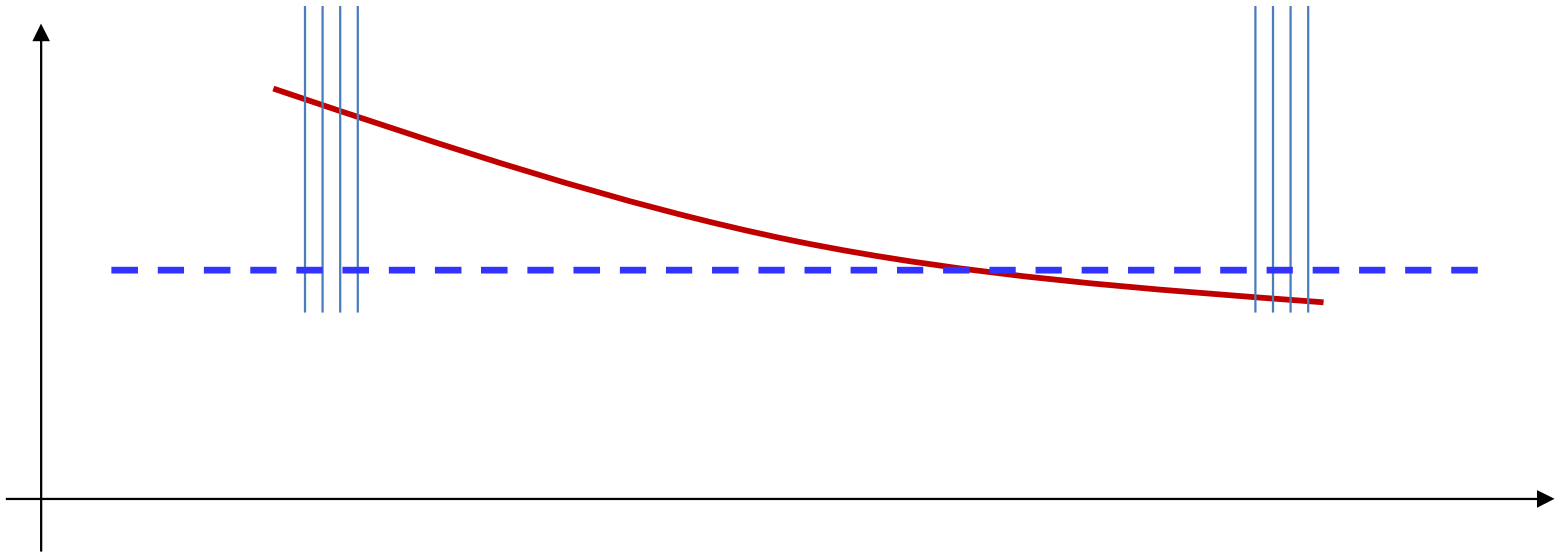

- If we loop through the samples in the same order, we may get *cyclic* behavior
- We must go through them *randomly* to get more convergent behavior

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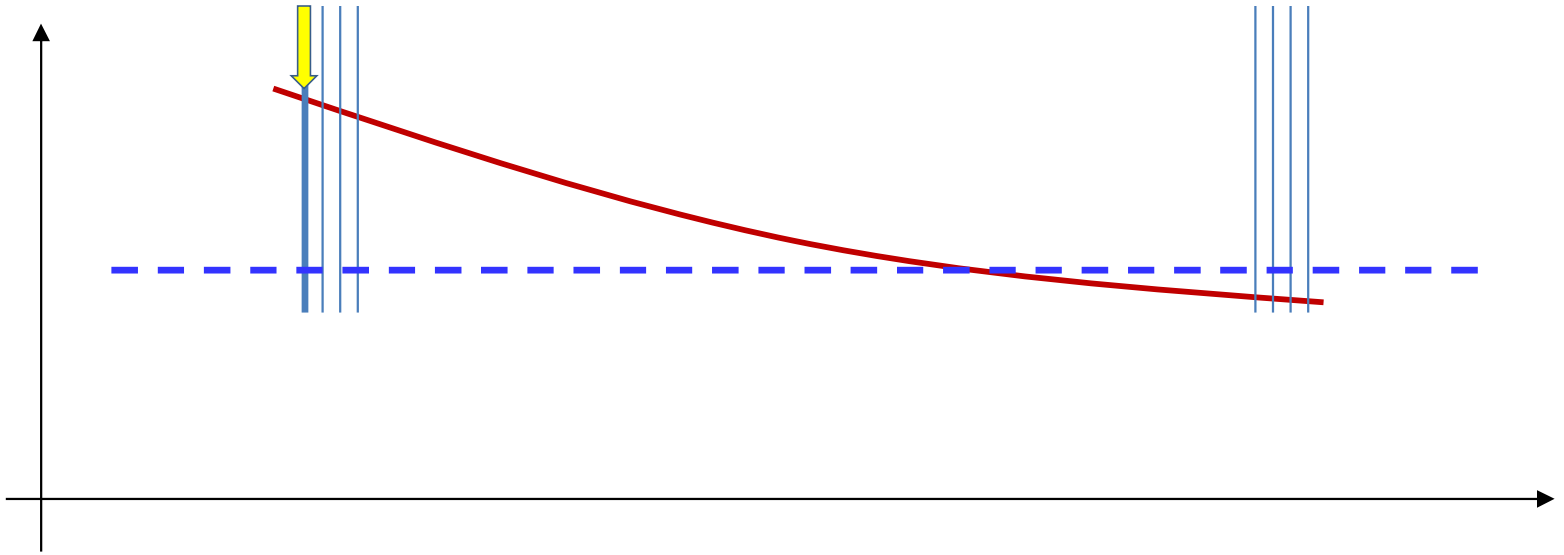

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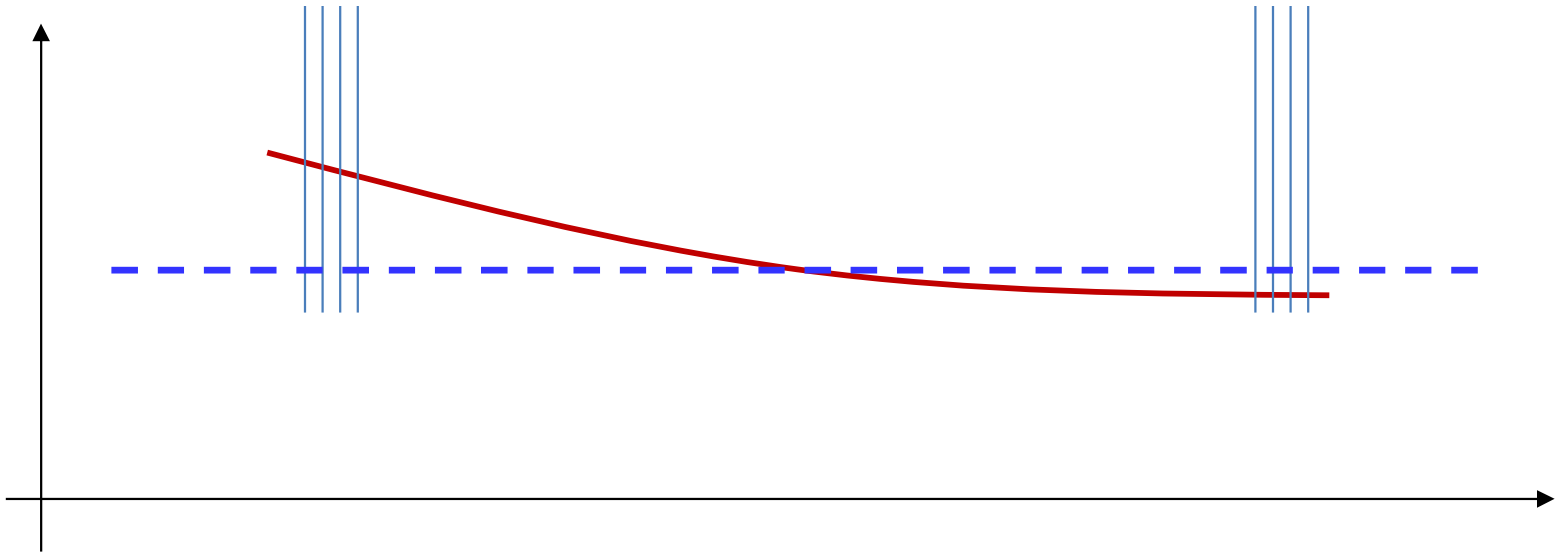

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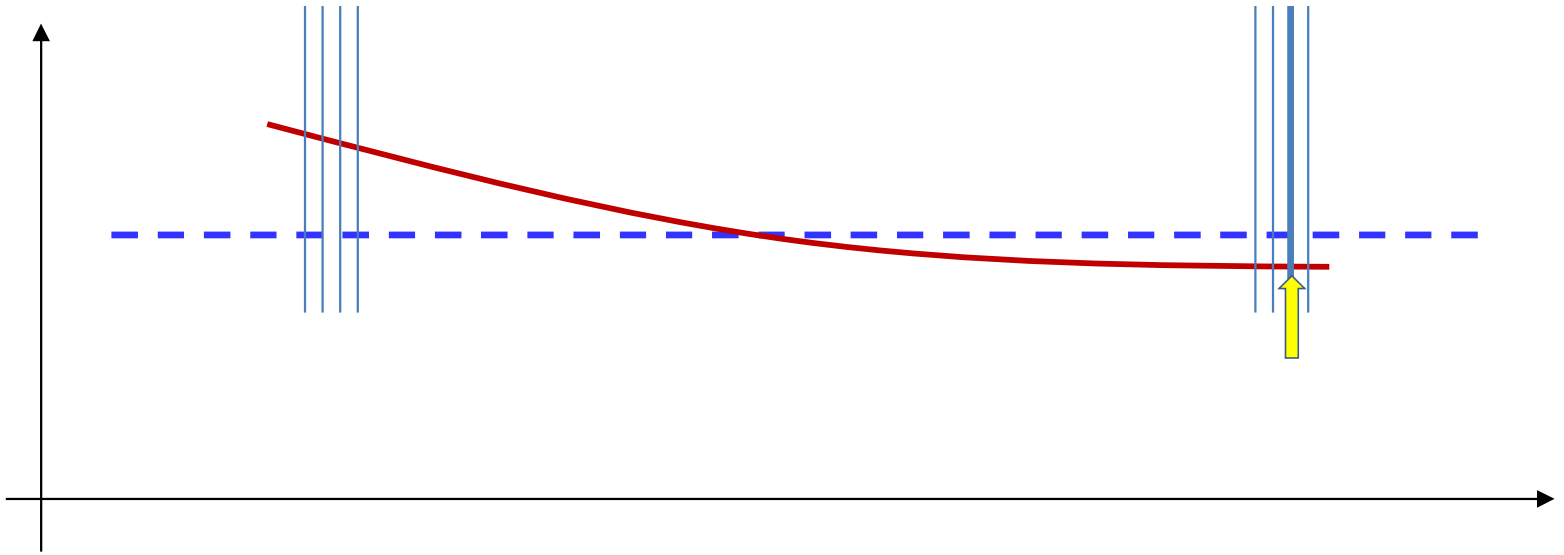

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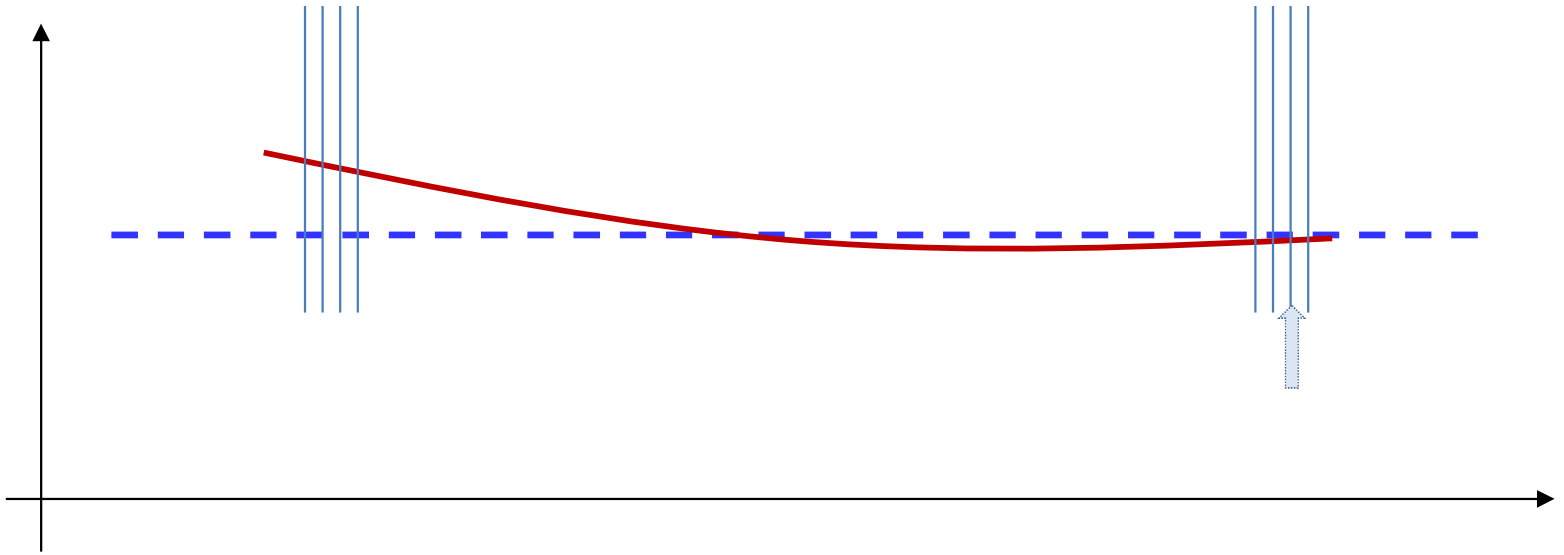

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Incremental Update: Stochastic Gradient Descent

- Given $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- Initialize all weights $W_1, W_2, \ldots, W_K$
- Do:
  - Randomly permute $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
  - For all $t = 1:T$
    - For every layer k:
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$$W_k = W_k - \eta \nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})^T$$

- Until $Loss$ has converged

Story so far

- In any gradient descent optimization problem, presenting training instances incrementally can be more effective than presenting them all at once
  - Provided training instances are provided in random order
  - "Stochastic Gradient Descent"
- This also holds for training neural networks

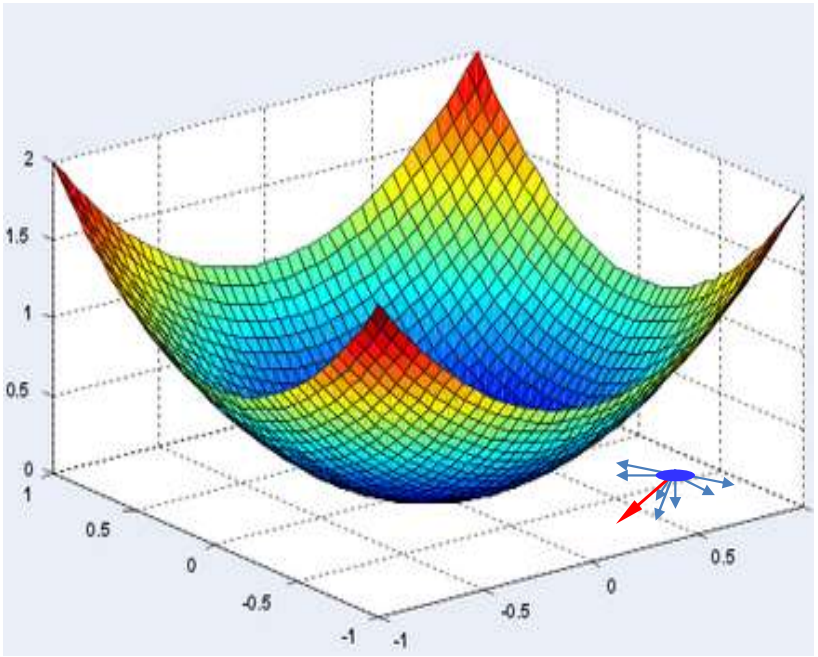
Explanations and restrictions

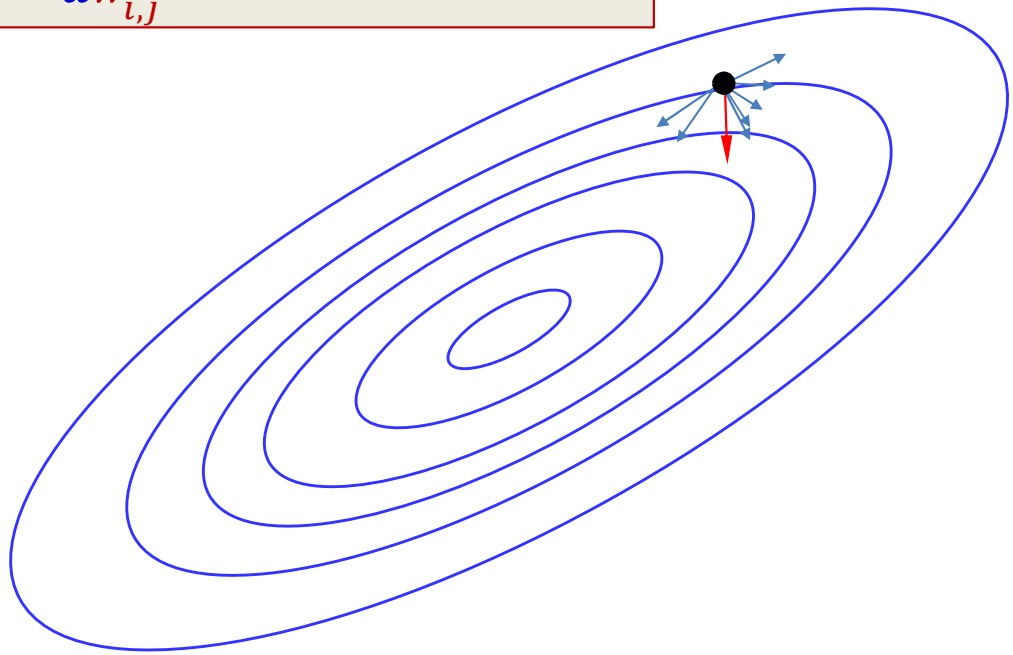
- So why does this process of incremental updates work?
- Under what conditions?

- For “why”: first consider a simplistic explanation that’s often given
  - Look at an extreme example

The expected behavior of the gradient

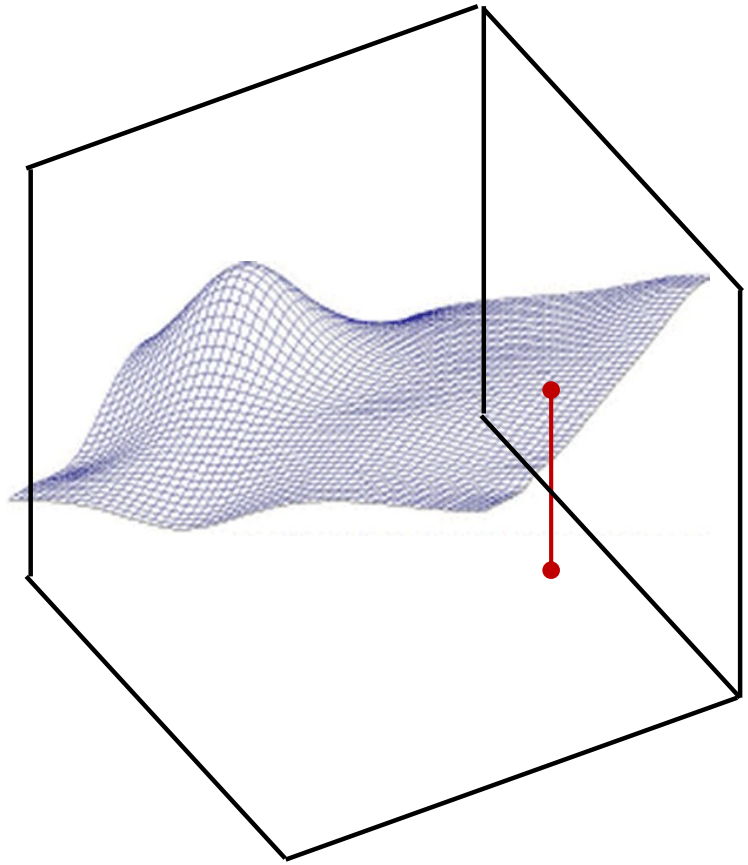
$$\frac{dE(\boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}, \ldots, \boldsymbol{W}^{(K)})}{\boldsymbol{d}w_{i,j}^{(k)}} = \frac{1}{T}\sum_{i} \frac{\boldsymbol{dDiv}(\boldsymbol{Y}(\boldsymbol{X_i}), \boldsymbol{d_i}; \boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}, \ldots, \boldsymbol{W}^{(K)})}{\boldsymbol{d}w_{i,j}^{(k)}}$$





- The individual training instances contribute different directions to the overall gradient
  - The final gradient points is the average of individual gradients
  - It points towards the *net* direction

Extreme example

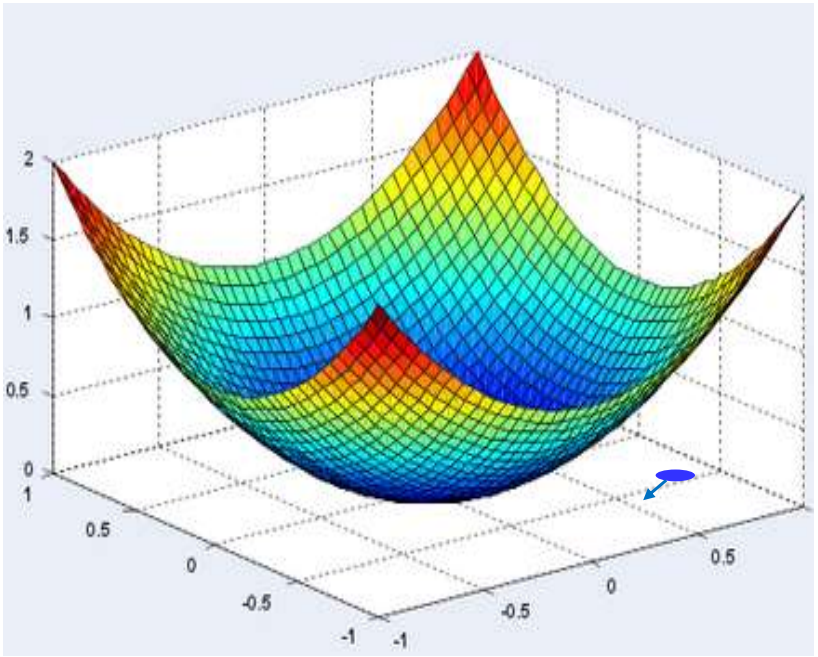


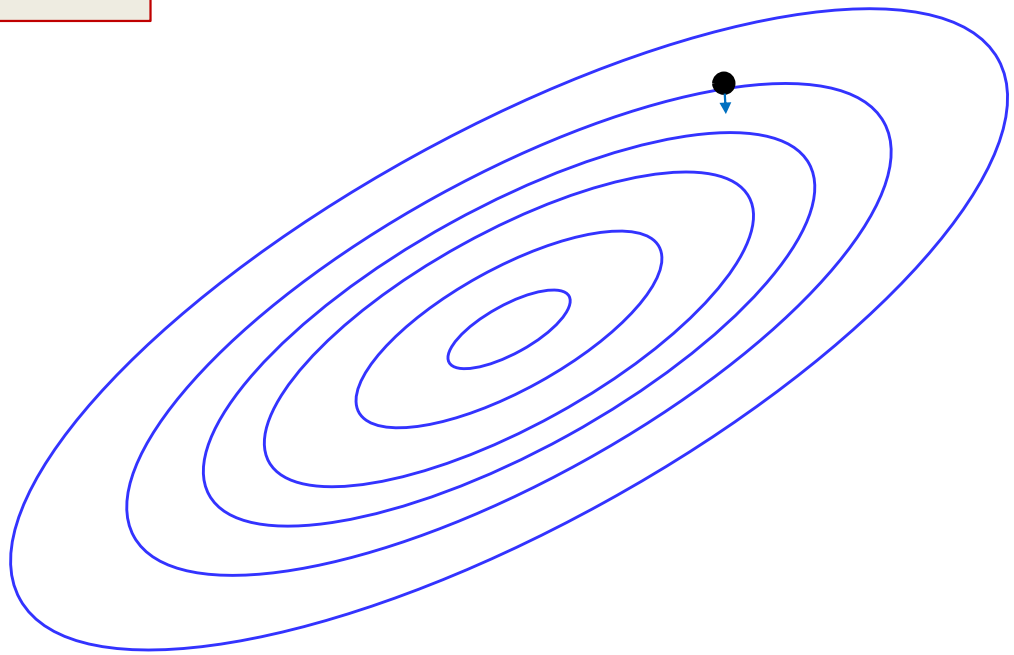
$$X_1 = X_2 = \cdots = X_T$$

- Extreme instance of data clotting: all the training instances are exactly the same

The expected behavior of the gradient

$$\frac{dE}{dw_{i,j}^{(k)}} = \frac{1}{T}\sum_{i}\frac{dDiv(Y(X_i), d_i)}{dw_{i,j}^{(k)}} = \frac{dDiv(Y(X_i), d_i)}{dw_{i,j}^{(k)}}$$

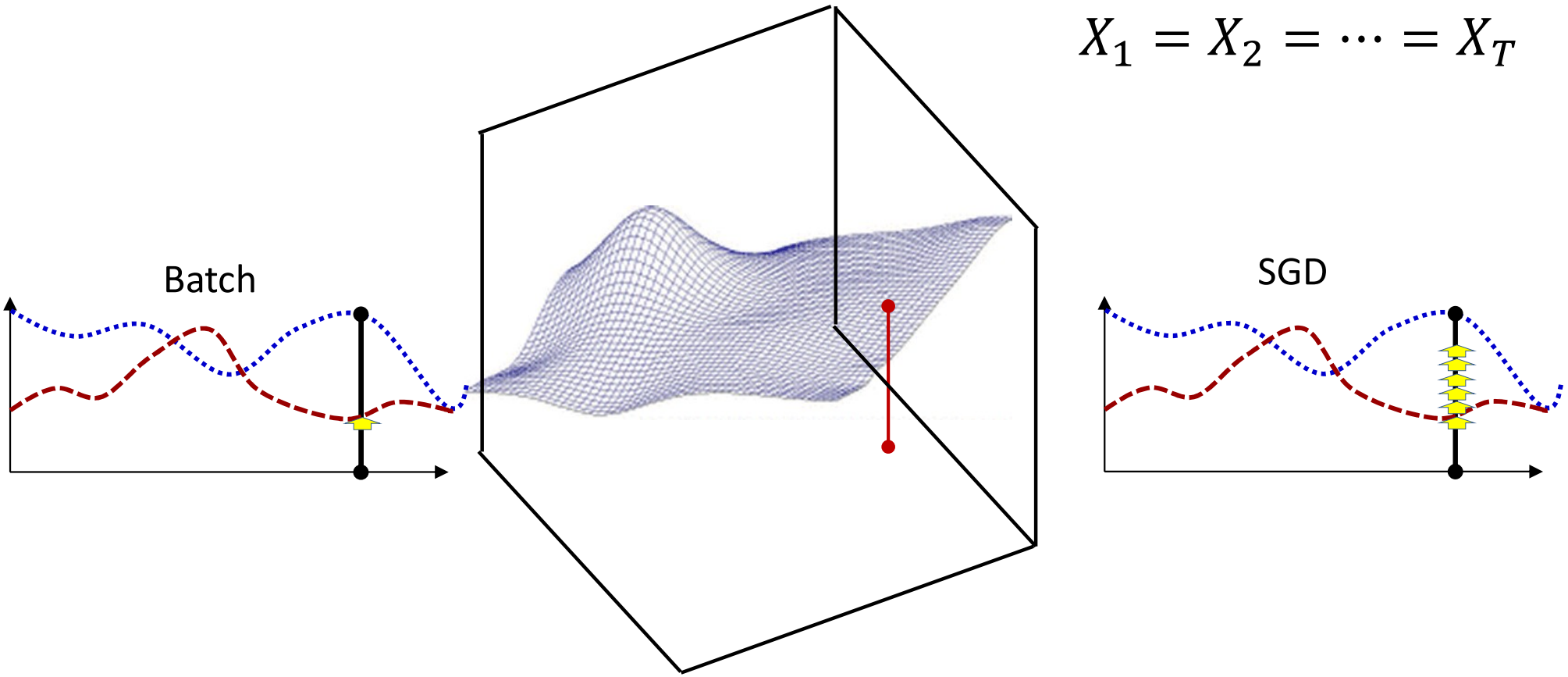




- The individual training instance contribute identical directions to the overall gradient
  - The final gradient points is simply the gradient for an individual instance

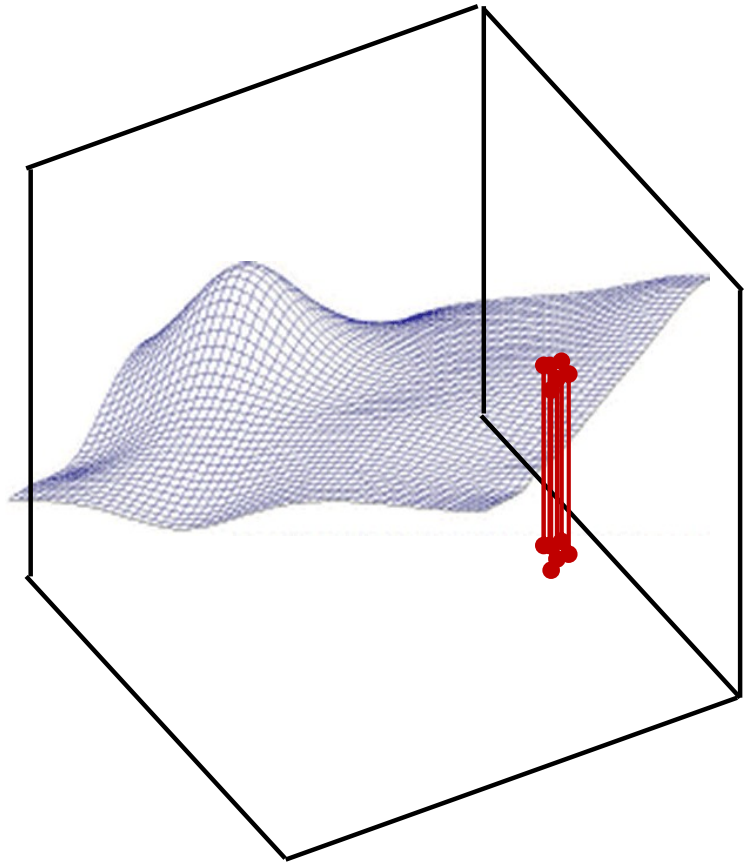
Batch vs SGD

$$X_1 = X_2 = \cdots = X_T$$



- Batch gradient descent operates over *T* training instances to get a *single* update
- SGD gets T updates for the same computation

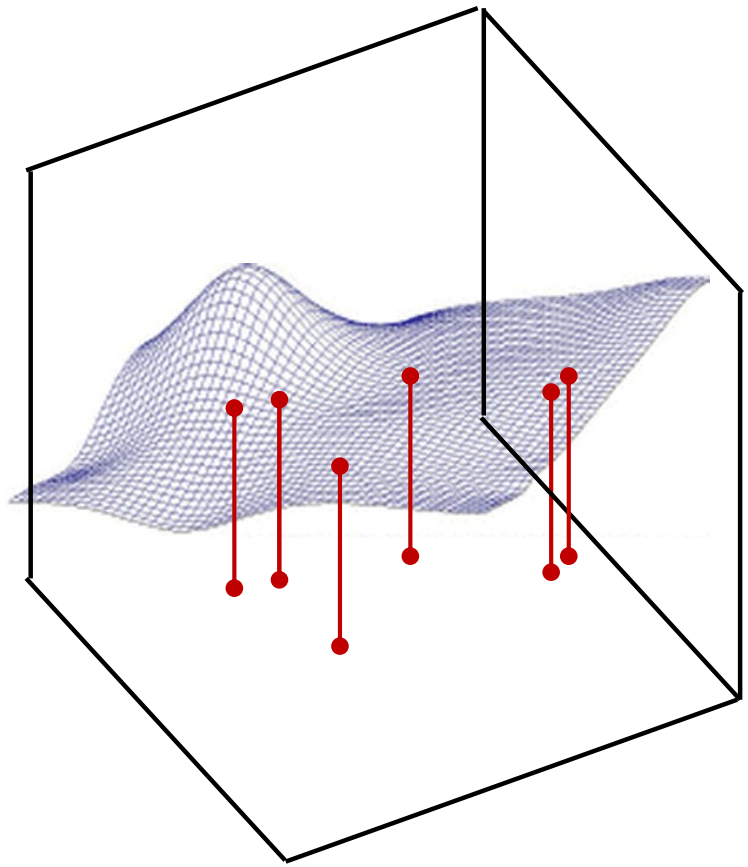
Clumpy data..



$$X_1 \approx X_2 \approx \cdots \approx X_T$$

- Also holds if all the data are not identical, but are tightly clumped together

Clumpy data..

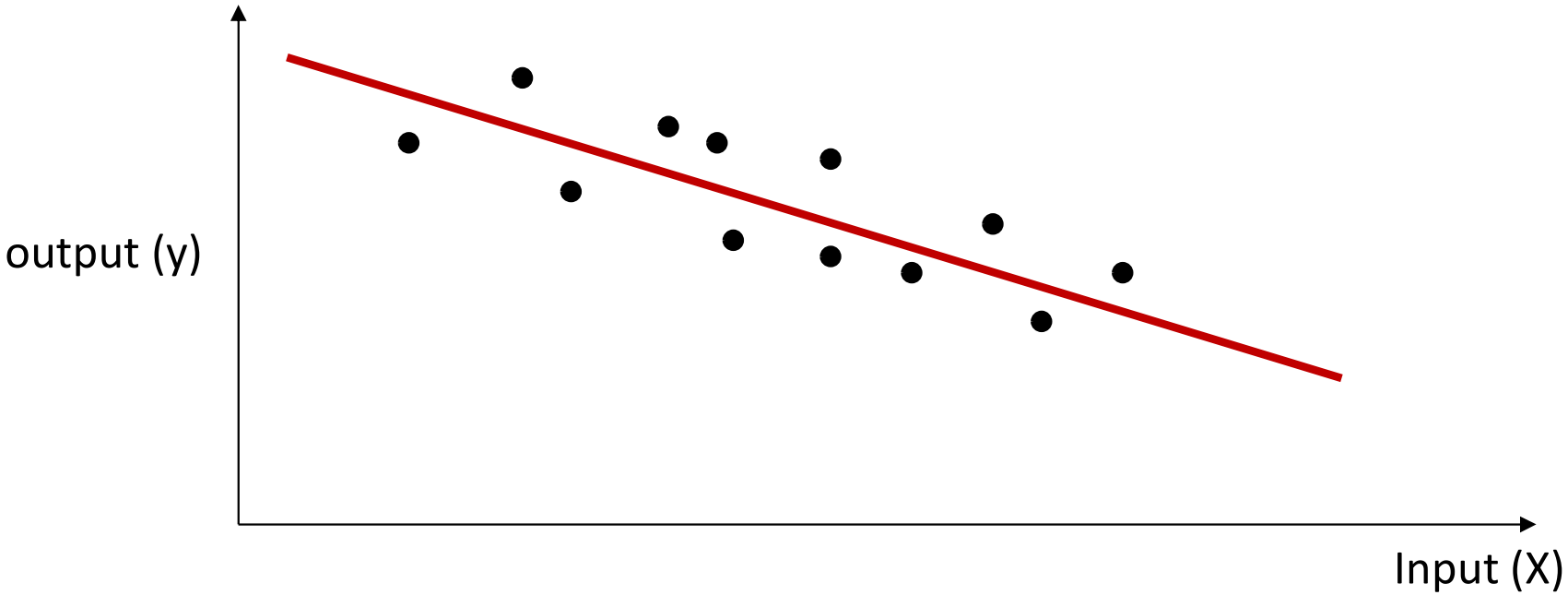


- As data get increasingly diverse, the benefits of incremental updates decrease, but do not entirely vanish

When does it work

- What are the considerations?
- And how well does it work?

Caveats: learning rate



- Except in the case of a perfect fit, even an optimal overall fit will look incorrect to *individual* instances
  - Correcting the function for individual instances will lead to never-ending, non-convergent updates
  - We must *shrink* the learning rate with iterations to prevent this
    - Correction for individual instances with the eventual miniscule learning rates will not modify the function

Incremental Update: Stochastic Gradient Descent

- Given $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$
- Do:
  - Randomly permute $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
  - For all $t = 1:T$
    - $j = j + 1$
    - For every layer k:
      - Compute $\nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})$
      - Update

$$W_k = W_k - \eta_j \nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})^T$$

- Until $Loss$ has converged

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Randomize input order

Learning rate reduces with j

- Until $Loss$ has converged

SGD convergence

- SGD converges "almost surely" to a global or local minimum for most functions
  - Sufficient condition: step sizes follow the following conditions (Robbins and Munro 1951)

$$\sum_k \eta_k = \infty$$

    - Eventually the entire parameter space can be searched

$$\sum_k \eta_k^2 < \infty$$

    - The steps shrink
  - The fastest converging series that satisfies both above requirements is

$$\eta_k \propto \frac{1}{k}$$

    - This is the optimal rate of shrinking the step size for strongly convex functions
  - More generally, the learning rates are heuristically determined
- If the loss is convex, SGD converges to the optimal solution
- For non-convex losses SGD converges to a local minimum

SGD convergence

- We will define convergence in terms of the number of iterations taken to get within ϵ of the optimal solution
  - $\left|f\left(W^{(k)}\right) - f(W^*)\right| < \epsilon$
  - Note: $f(W)$ here is the optimization objective on the *entire* training data, although SGD itself updates after every training instance

- Using the optimal learning rate $1/k$, for *strongly convex* functions,

$$\left|f\left(W^{(k)}\right) - f(W^*)\right| < \frac{1}{k}\left|f\left(W^{(0)}\right) - f(W^*)\right|$$

  - Strongly convex → Can be placed inside a quadratic bowl, touching at any point
  - Giving us the iterations to ϵ convergence as $O\left(\frac{1}{\epsilon}\right)$

- For generically convex (but not strongly convex) function, various proofs report an ϵ convergence of $\frac{1}{\sqrt{k}}$ using a learning rate of $\frac{1}{\sqrt{k}}$.

Batch gradient convergence

- In contrast, using the batch update method, for *strongly convex* functions,

$$\left|f\left(W^{(k)}\right) - f(W^*)\right| < c^k \left|f\left(W^{(0)}\right) - f(W^*)\right|$$

  - Giving us the iterations to ϵ convergence as $O\left(log\left(\frac{1}{\epsilon}\right)\right)$

- For generic convex functions, iterations to ϵ convergence is $O\left(\frac{1}{\epsilon}\right)$

- Batch gradients converge "faster"
  - But SGD performs T updates for every batch update

SGD Convergence: Loss value

If:

- f is λ-strongly convex, and
- at step t we have a noisy estimate of the subgradient $\hat{g}_t$ with $\mathbb{E}[\|\hat{g}_t\|^2] \leq G^2$ for all t,
- and we use step size $\eta_t = {}^1/_{\lambda t}$

Then for any $T > 1$:

$$\mathbb{E}[f(w_T) - f(w^*)] \leq \frac{17G^2(1 + \log(T))}{\lambda T}$$

SGD Convergence

- We can bound the expected difference between the loss over our data using the optimal weights w^* and the weights w_T at any single iteration to $\mathcal{O}\left(\frac{\log(T)}{T}\right)$ for strongly convex loss or $\mathcal{O}\left(\frac{\log(T)}{\sqrt{T}}\right)$ for convex loss

- Averaging schemes can improve the bound to $\mathcal{O}\left(\frac{1}{T}\right)$ and $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$

- Smoothness of the loss is not required

SGD Convergence and weight averaging

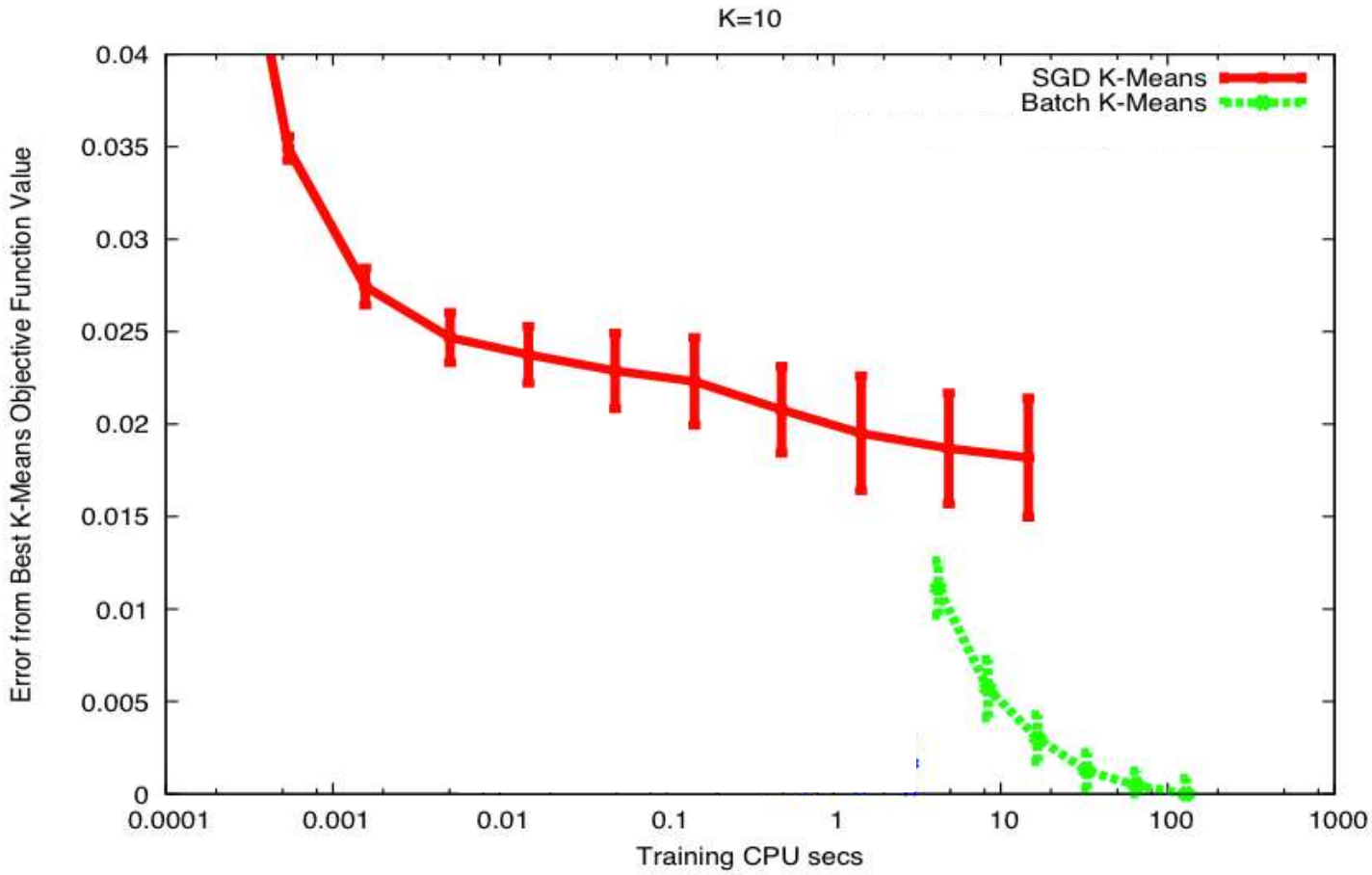
Polynomial Decay Averaging:

$$\bar{w}_t^{\gamma} = \left(1 - \frac{\gamma + 1}{t + \gamma}\right) \bar{w}_{t-1}^{\gamma} + \frac{\gamma + 1}{t + \gamma} w_t$$

With γ some small positive constant, e.g. $\gamma = 3$

Achieves $\mathcal{O}\left(\frac{1}{T}\right)$ (strongly convex) and $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ (convex) convergence

SGD example



- A simpler problem: K-means
- Note: SGD converges faster
  - But to a poorer minimum
- Also note the rather large variation between runs
  - Let's try to understand these results..

Poll 2

PIAZZA @529

Select all that are true

- SGD is an online version of batch updates
- SGD can have oscillatory behavior if we do not randomize the order of the inputs
- SGD can converge faster than batch updates, but arrive at poorer optima
- SGD convergence to the global optimum can only be guaranteed if step sizes shrink across iterations, but sum to infinity in the limit

Poll 2

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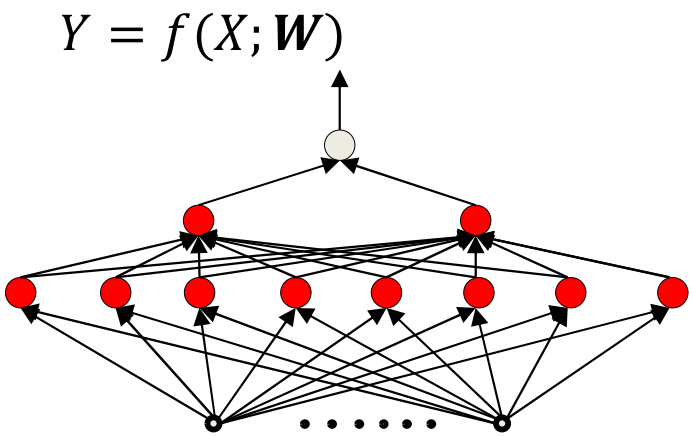
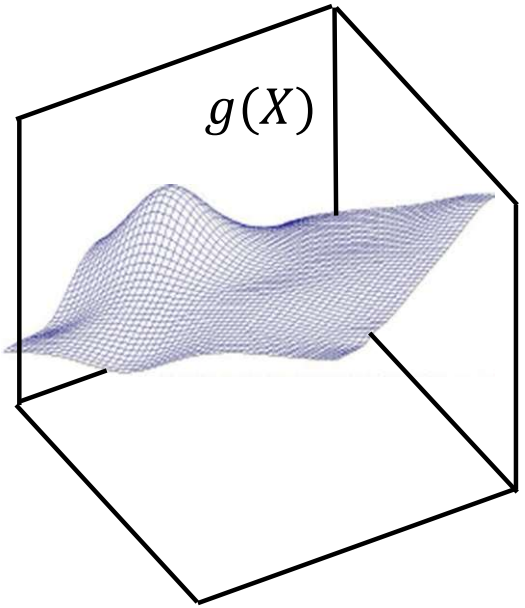
Recall: Modelling a function



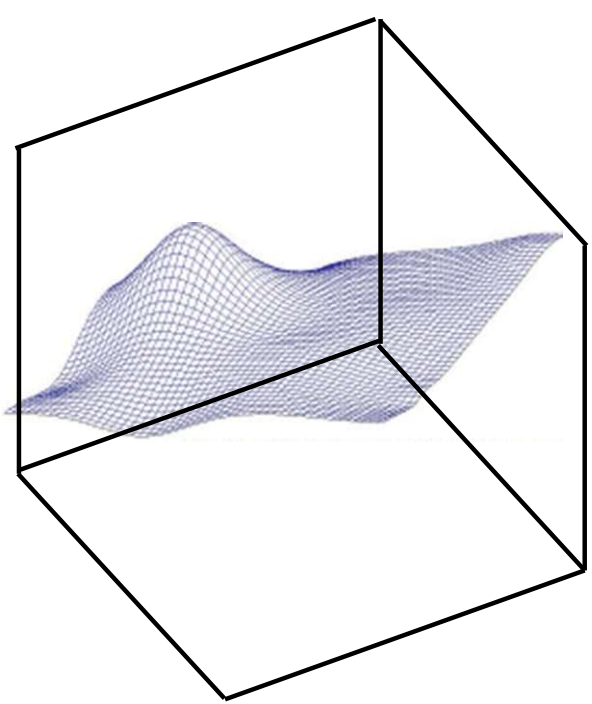


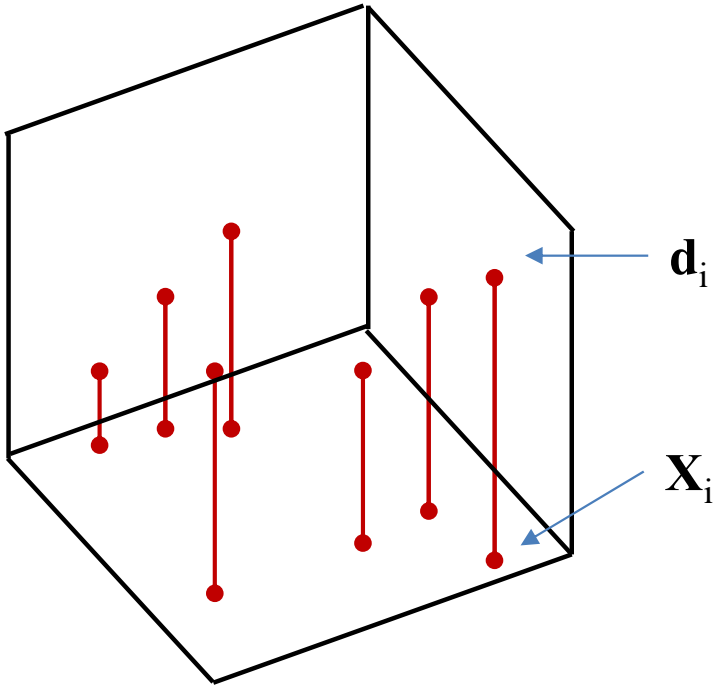
- To learn a network $f(X; \boldsymbol{W})$ to model a function $g(X)$ we minimize the *expected divergence*

$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}} \int_X div\big(f(X; W), g(X)\big) P(X) dX$$

$$= \underset{W}{\operatorname{argmin}}\, E\big[div\big(f(X; W), g(X)\big)\big]$$

Recall: The *Empirical* risk





- In practice, we minimize the *empirical risk (or loss)*

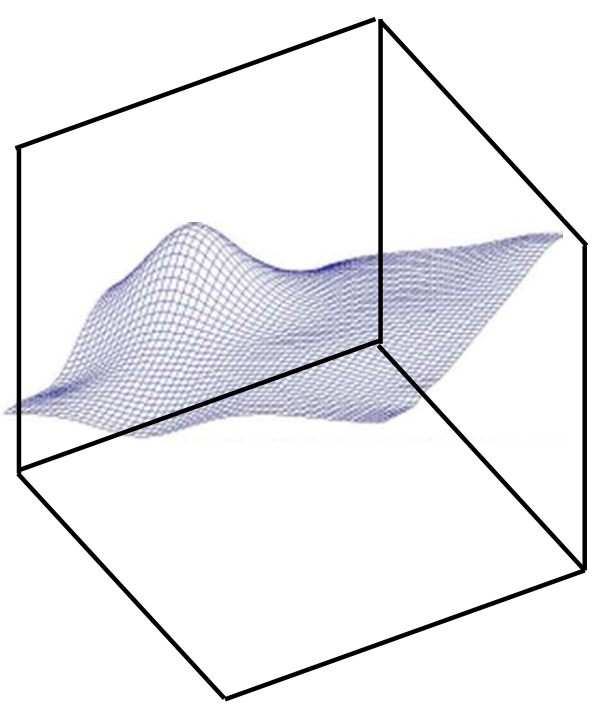
$$Loss(W) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i; W), d_i)$$

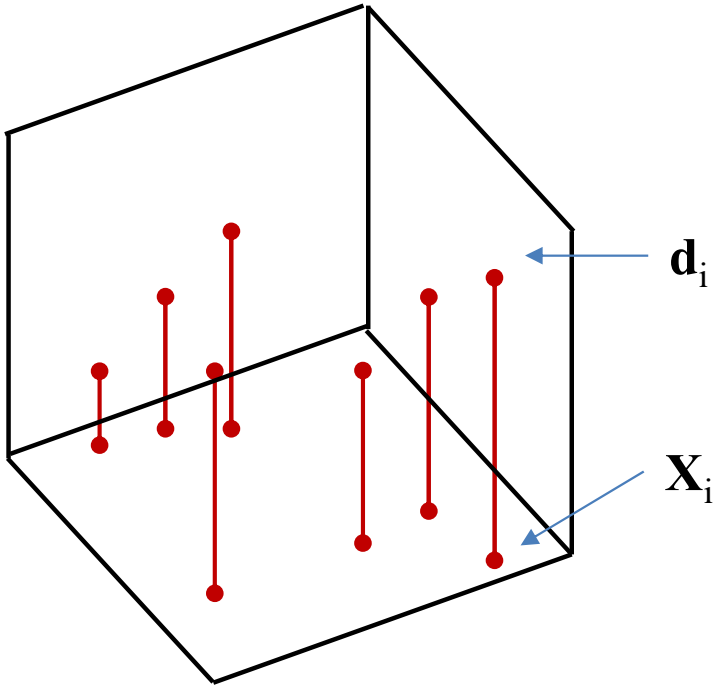
$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}}\, Loss(W)$$

- The *expected value* of the *empirical risk* is actually the *expected divergence*

$$E[Loss(W)] = E\left[div\left(f(X; W), g(X)\right)\right]$$

Recall: The *Empirical* risk





- In practice, we minimize the *empirical risk (or loss)*

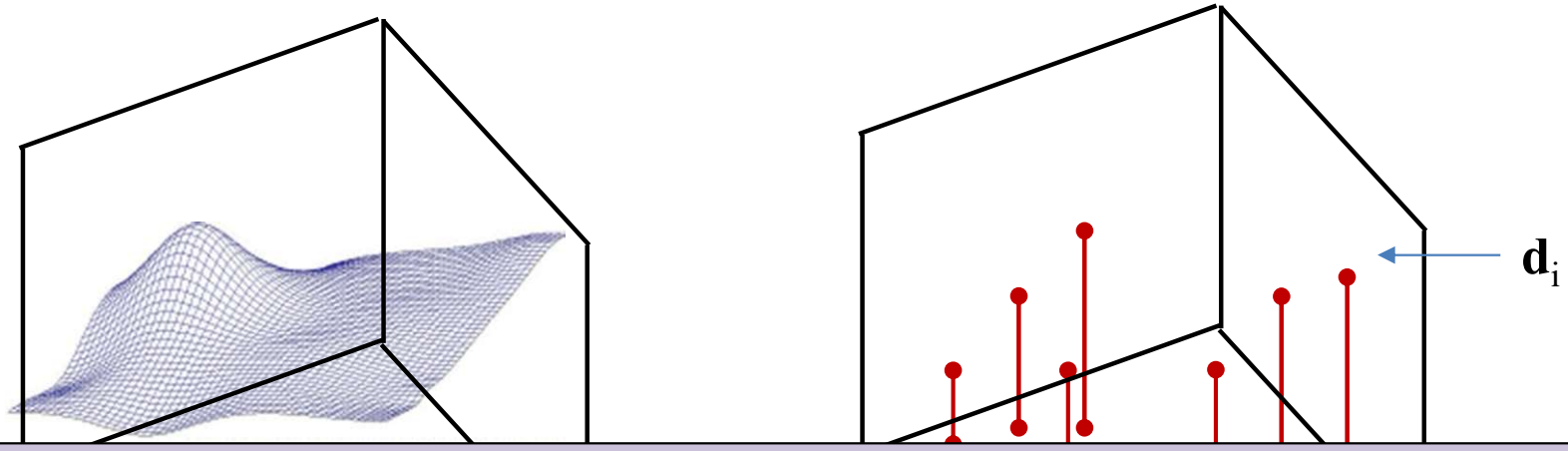
$$Loss(W) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i; W), d_i)$$

The empirical risk is an *unbiased* estimate of the expected divergence

Though there is no guarantee that minimizing it will minimize the expected divergence

$$E[Loss(W)] = E\big[div\big(f(X; W), g(X)\big)\big]$$

Recall: The *Empirical* risk



The variance of the empirical risk: var(Loss) = 1/N var(div)

The variance of the estimator is proportional to 1/N

The larger this variance, the greater the likelihood that the W that minimizes the empirical risk will differ significantly from the W that minimizes the expected divergence

$$Loss(W) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i; W), d_i)$$

The empirical risk is an *unbiased* estimate of the expected divergence

Though there is no guarantee that minimizing it will minimize the expected divergence

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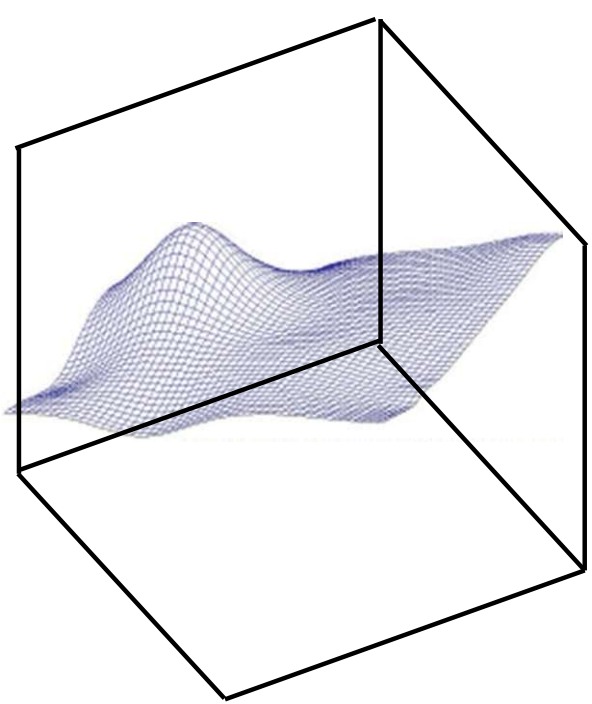
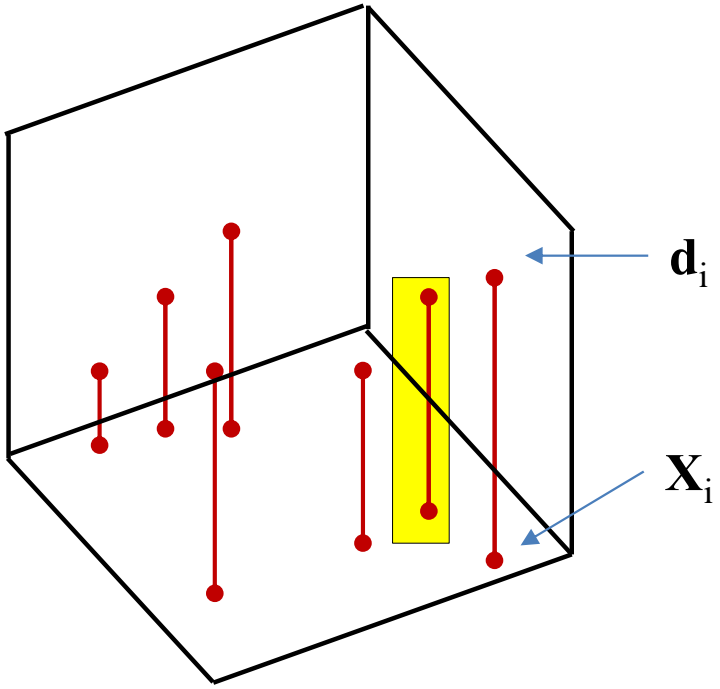
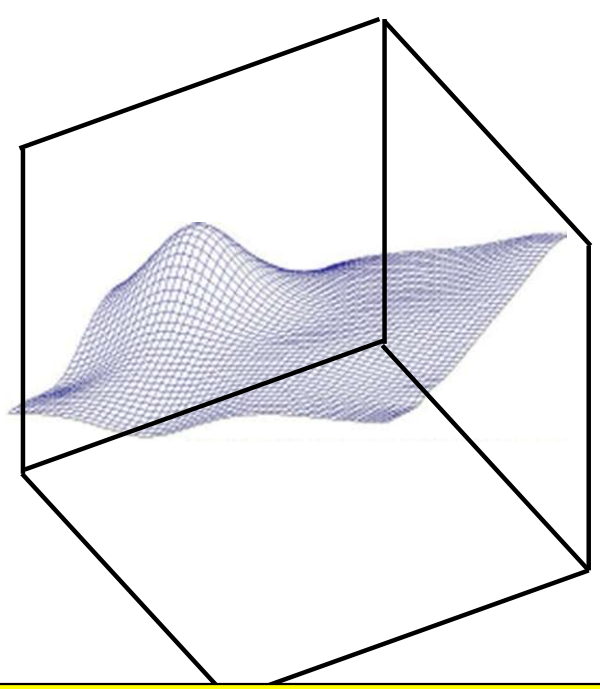
SGD

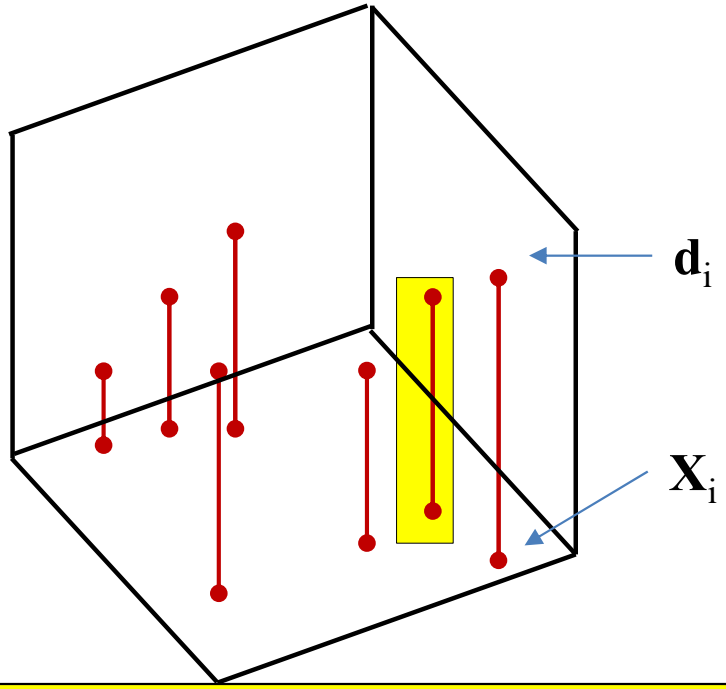




- At each iteration, **SGD** focuses on the divergence of a ***single*** sample $div(f(X_i; W), d_i)$
- The *expected value* of the *sample error* is ***still*** the *expected divergence* $E\left[div\left(f(X; W), g(X)\right)\right]$

SGD





The sample divergence is also an *unbiased* estimate of the expected error

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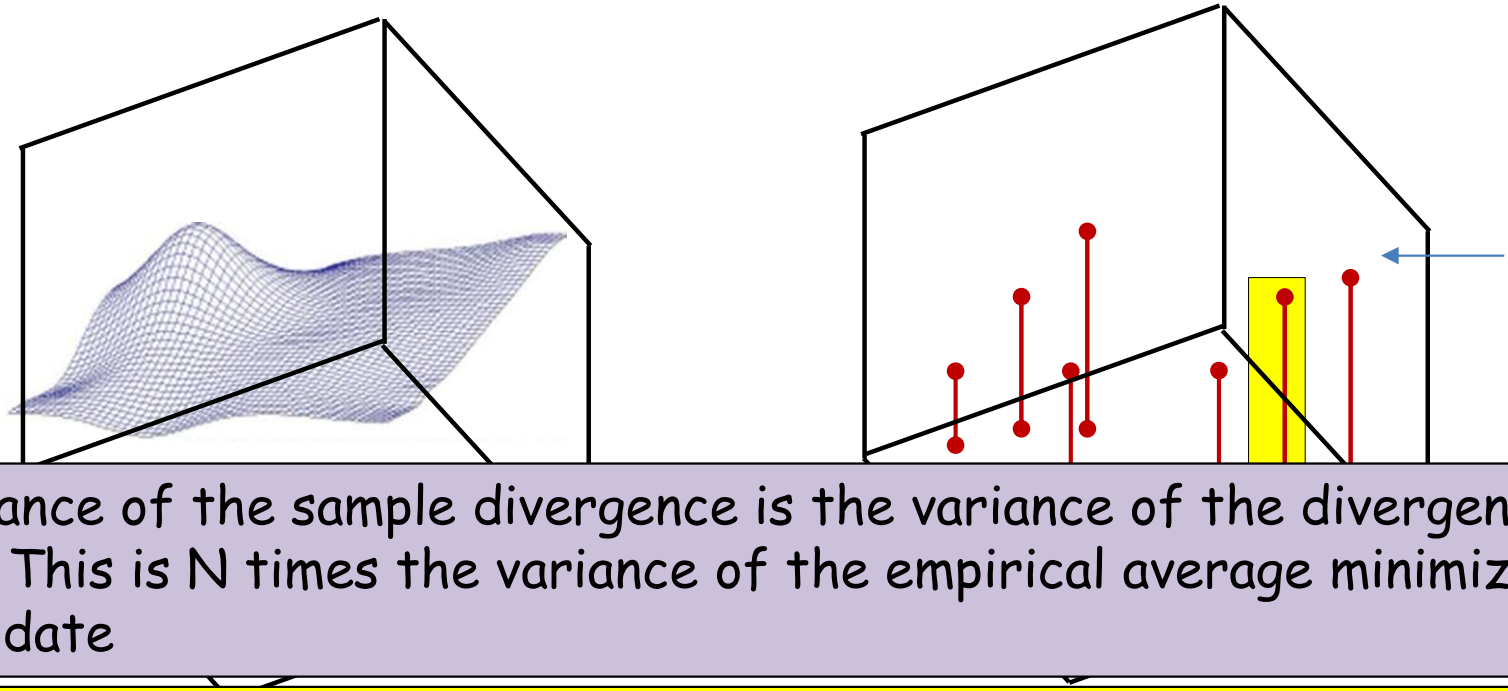
SGD



The variance of the sample divergence is the variance of the divergence itself: var(div). This is N times the variance of the empirical average minimized by batch update

The sample divergence is also an *unbiased* estimate of the expected error

- At each iteration, **SGD** focuses on the divergence of a ***single*** sample $div(f(X_i; W), d_i)$
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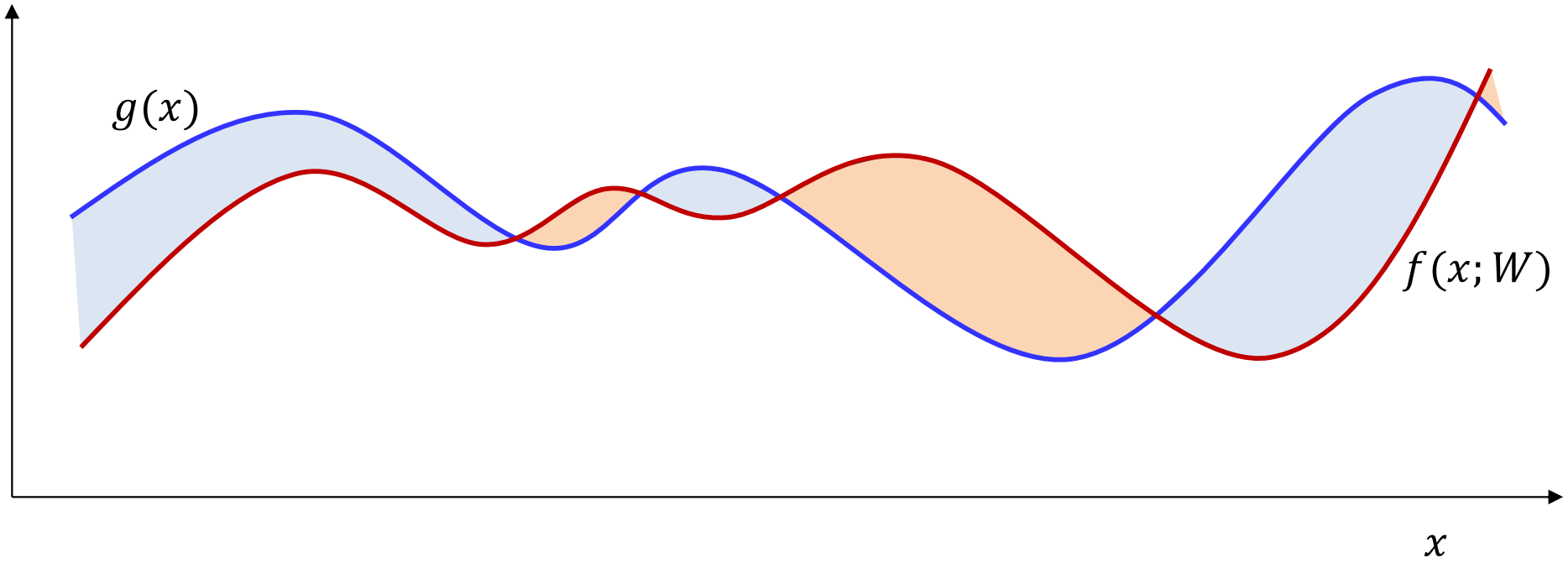
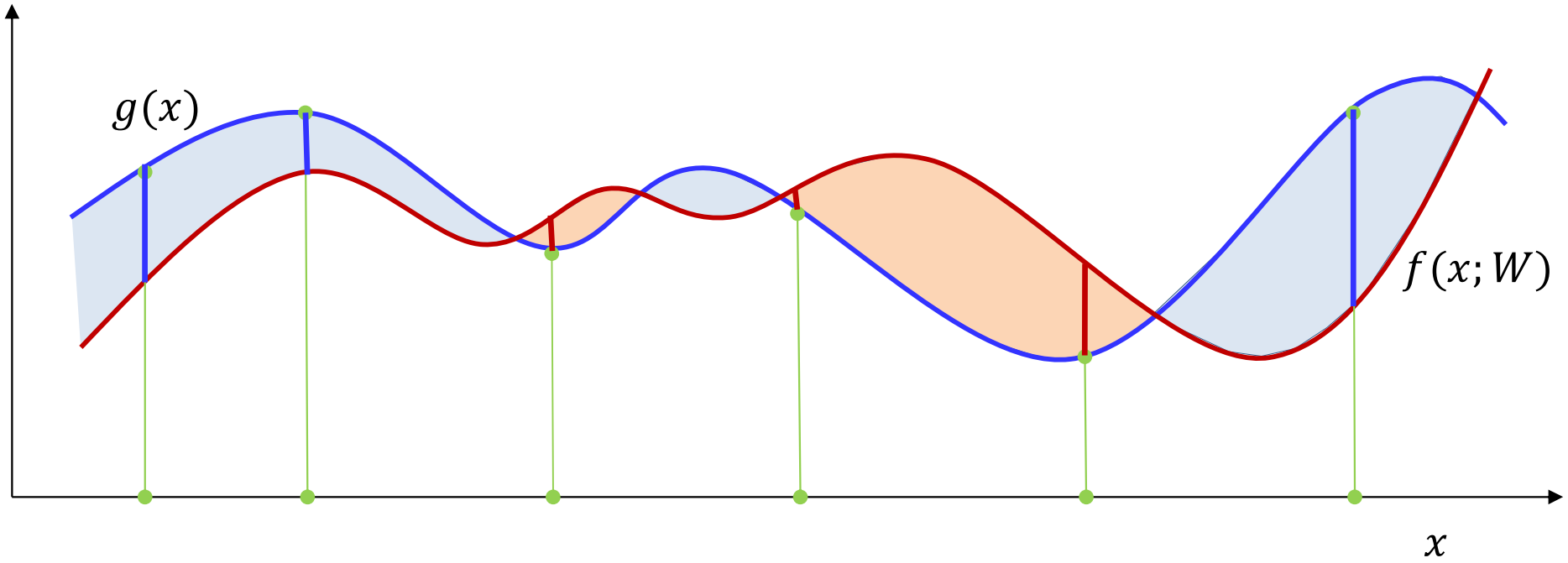
Explaining the variance



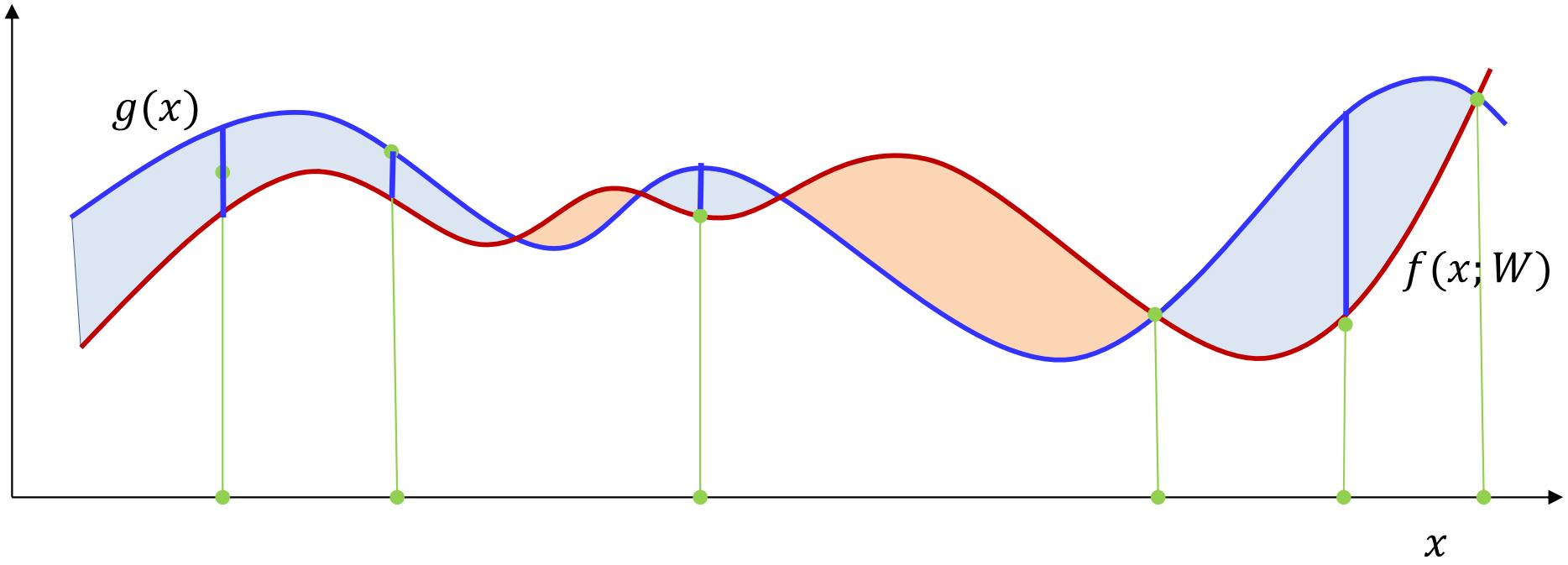
- The blue curve is the function being approximated
- The red curve is the approximation by the model at a given W
- The heights of the shaded regions represent the point-by-point error
  - The divergence is a function of the error
  - We want to find the W that minimizes the average divergence

Explaining the variance



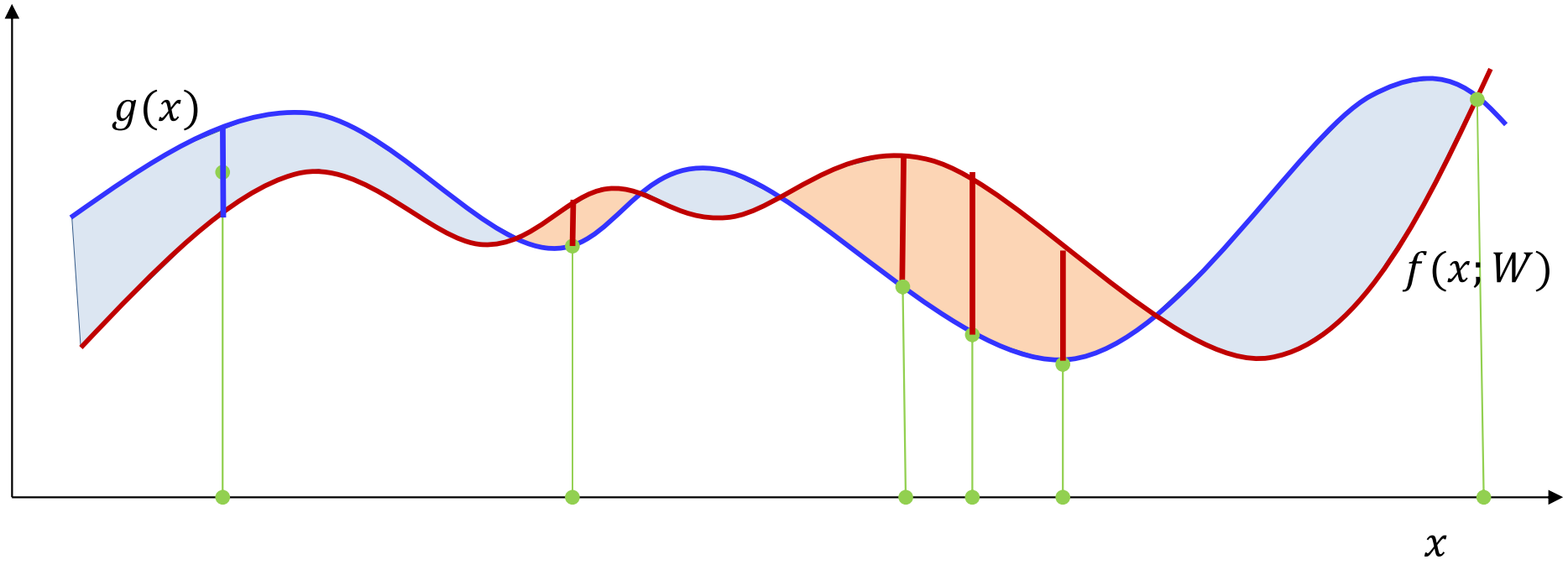
- Sample estimate approximates the shaded area with the average length of the lines

Explaining the variance



- Sample estimate approximates the shaded area with the average length of the lines
- This average length will change with position of the samples

Explaining the variance



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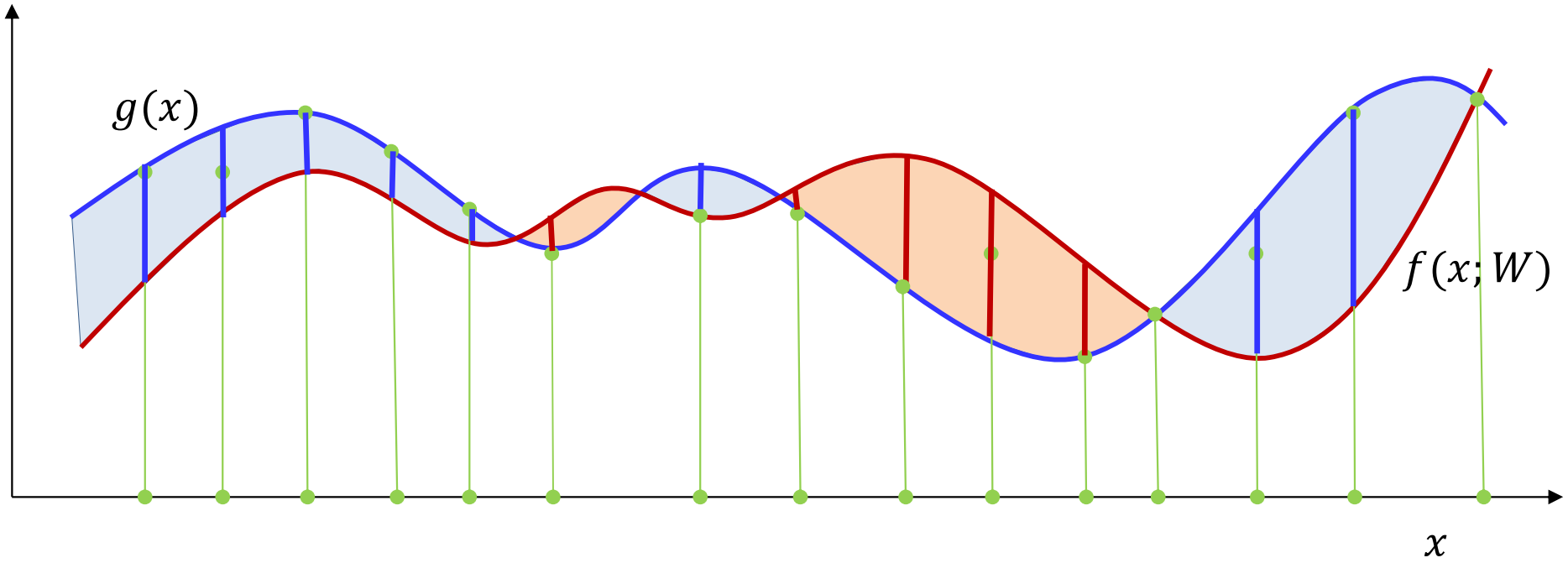
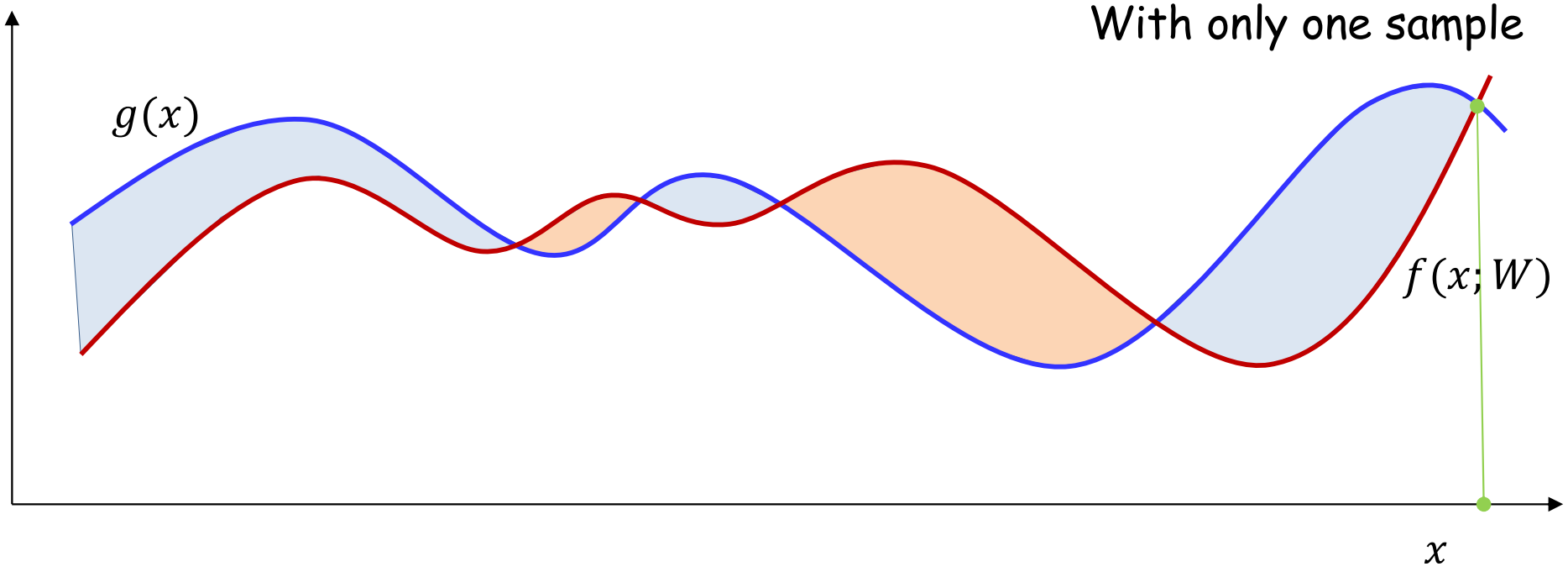


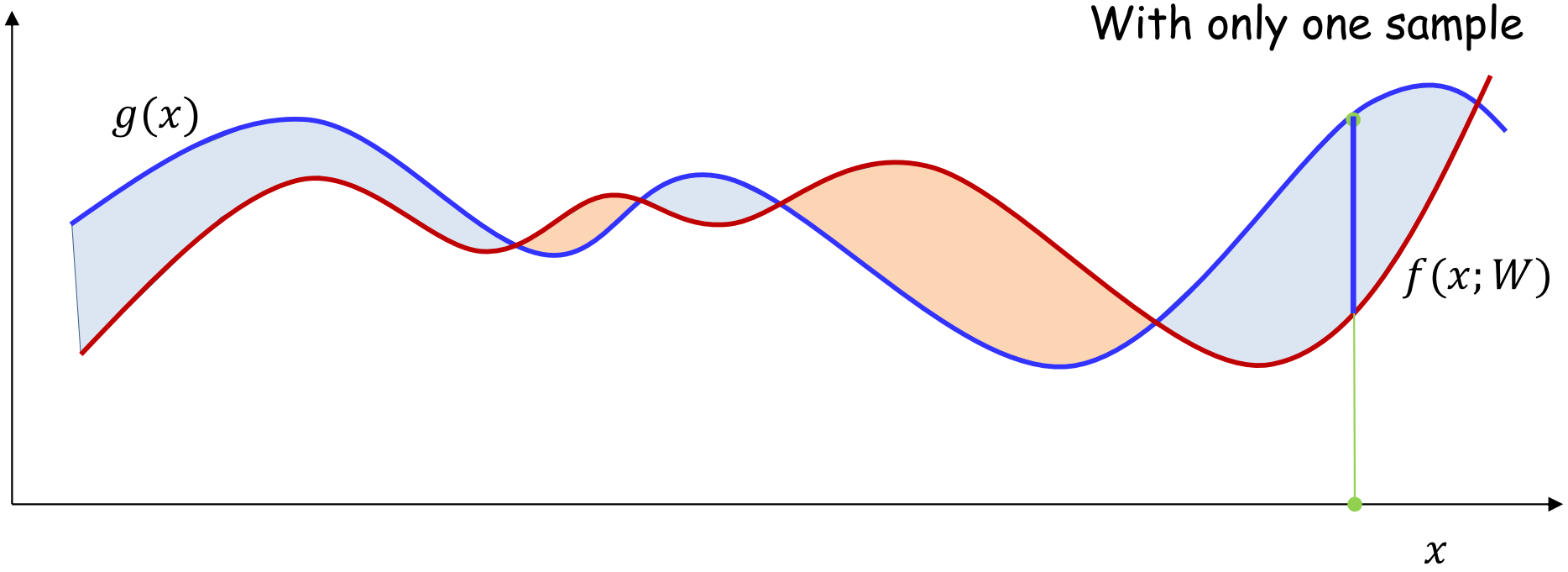
- Having more samples makes the estimate more robust to changes in the position of samples
  - The variance of the estimate is smaller

Explaining the variance



- Having very few samples makes the estimate swing wildly with the sample position
  - Since our estimator learns the W to minimize this estimate, the learned W too can swing wildly

Explaining the variance



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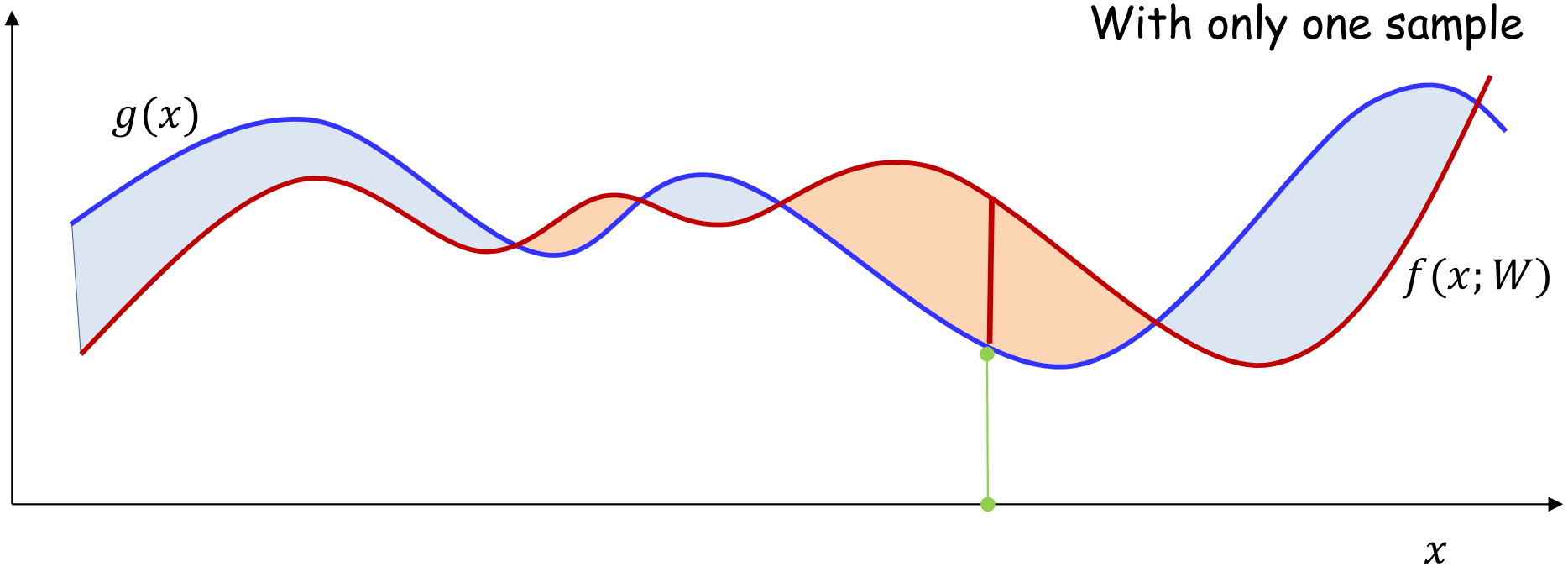

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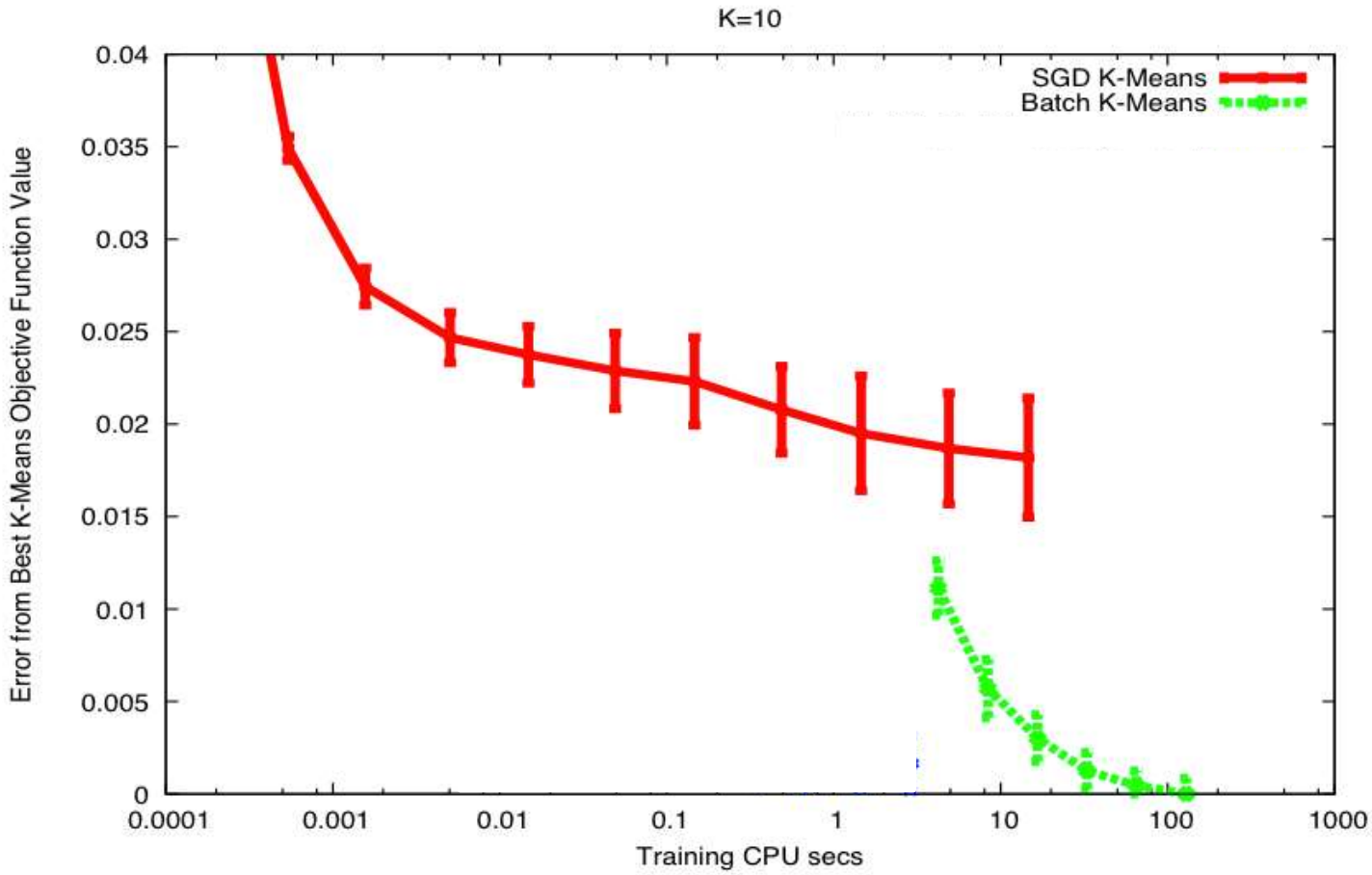
SGD example



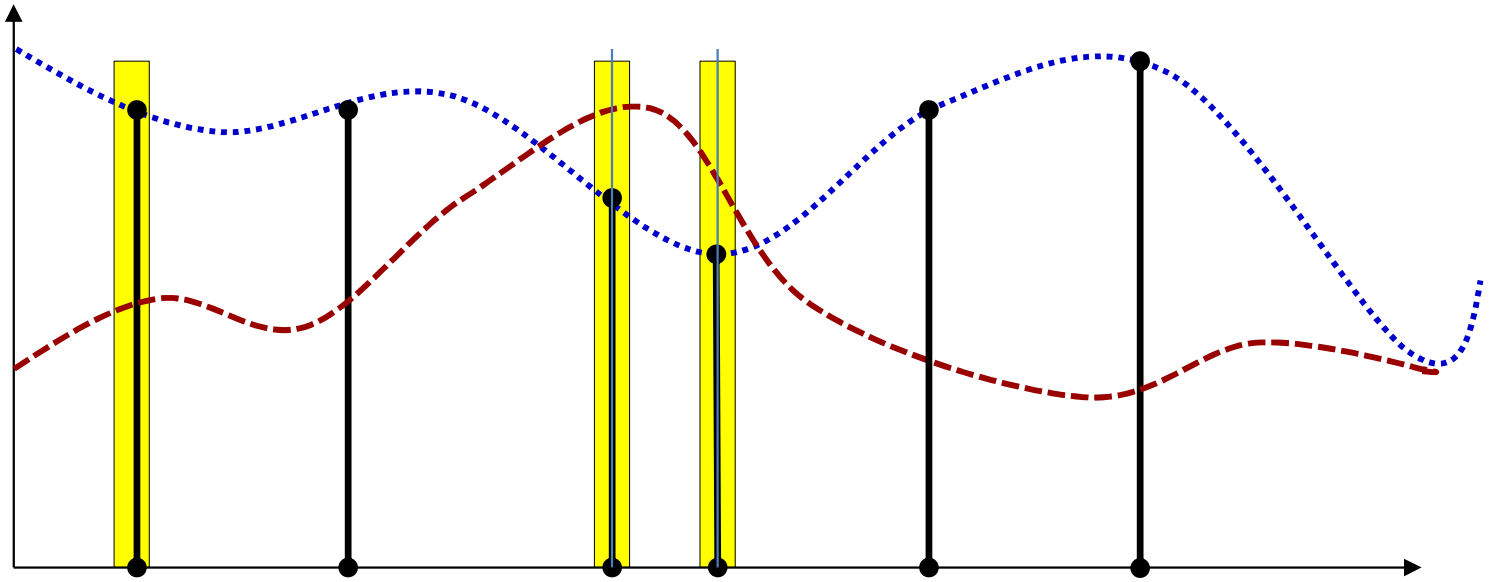
- A simpler problem: K-means
- Note: SGD converges faster
- But also has large variation between runs

SGD vs batch

- SGD uses the gradient from only one sample at a time, and is consequently high variance

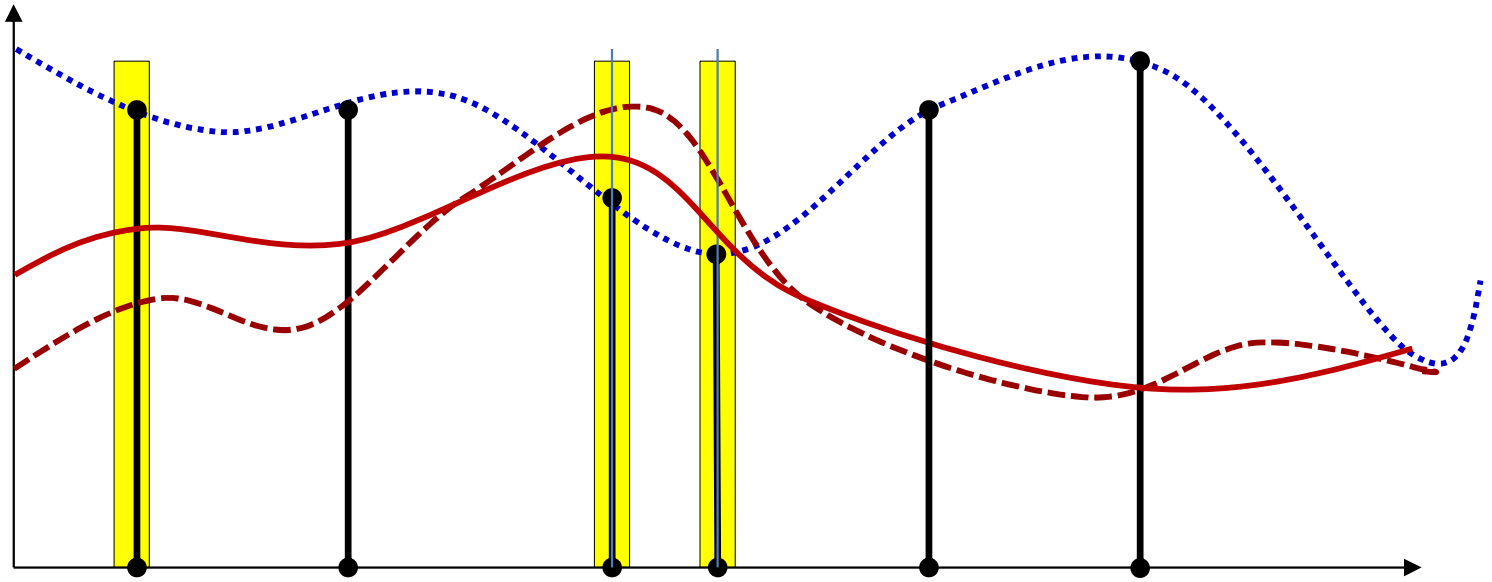
- But also provides significantly quicker updates than batch
- Is there a good medium?

Alternative: Mini-batch update



- Alternative: adjust the function at a small, randomly chosen subset of points
  - Keep adjustments small
  - If the subsets cover the training set, we will have adjusted the entire function
- As before, vary the subsets randomly in different passes through the training data

Alternative: Mini-batch update



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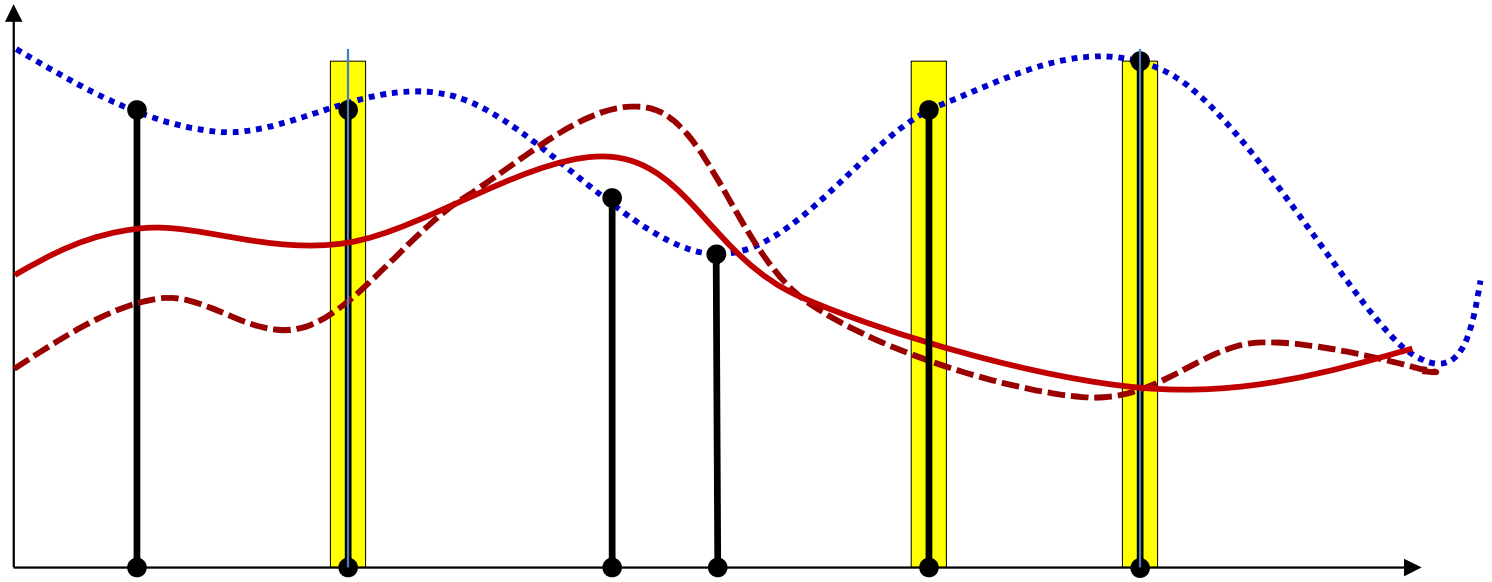

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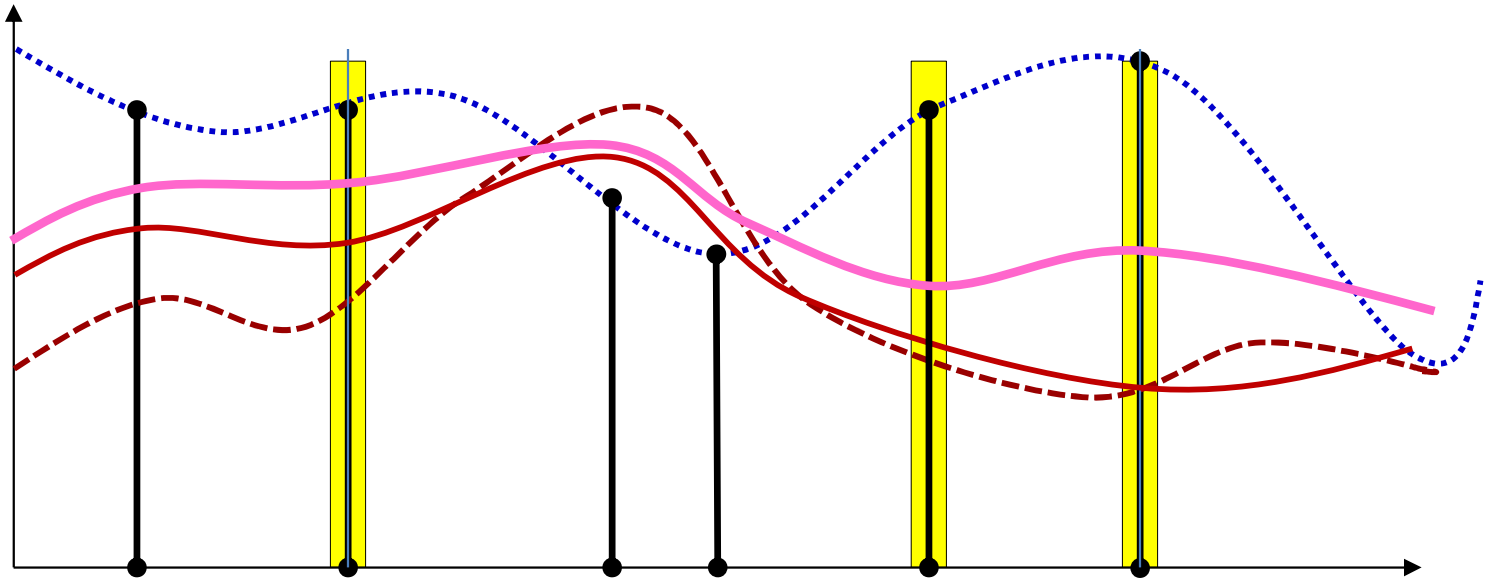

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Incremental Update: Mini-batch update

- Given $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$
- Do:
  - Randomly permute $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
  - For $t = 1 : b : T$
    - $j = j + 1$
    - For every layer k:
      - $\Delta W_k = 0$
    - For t' = t : t+b-1
      - For every layer k:
        - Compute $\nabla_{W_k} Div(Y_t, d_t)$
        - $\Delta W_k = \Delta W_k + \frac{1}{b} \nabla_{W_k} Div(Y_t, d_t)^T$
    - Update
      - For every layer k:

$$W_k = W_k - \eta_j \Delta W_k$$

- Until Err has converged

Incremental Update: Mini-batch update

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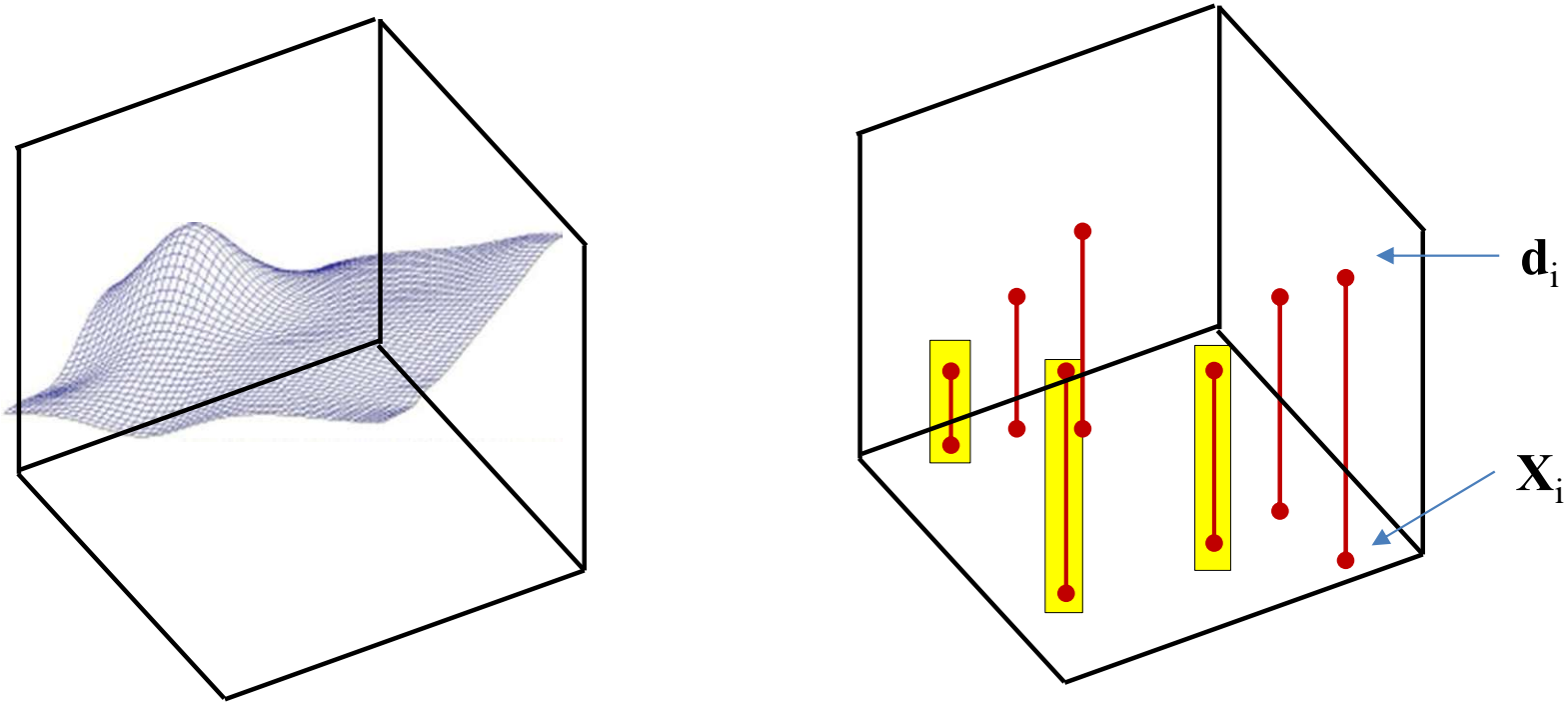
Mini-batch size

Shrinking step size

- Until Err has converged

Mini Batches



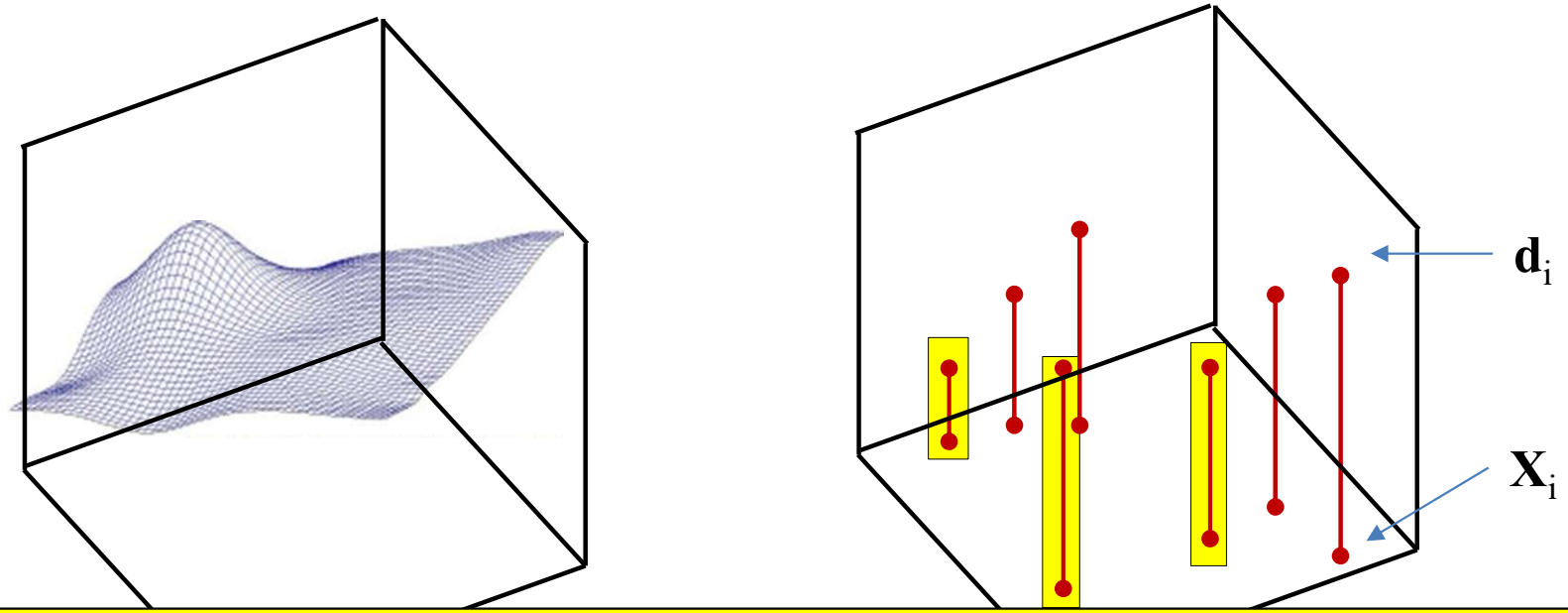
- Mini-batch updates compute and minimize a *batch loss*

$$MiniBatchLoss(W) = \frac{1}{b}\sum_{i=1}^{b} div(f(X_i; W), d_i)$$

- The *expected value* of the *batch loss* is also the *expected divergence*

$$E[MiniBatchLoss(W)] = E\left[div\left(f(X; W), g(X)\right)\right]$$

Mini Batches



The minibatch loss is also an unbiased estimate of the expected loss

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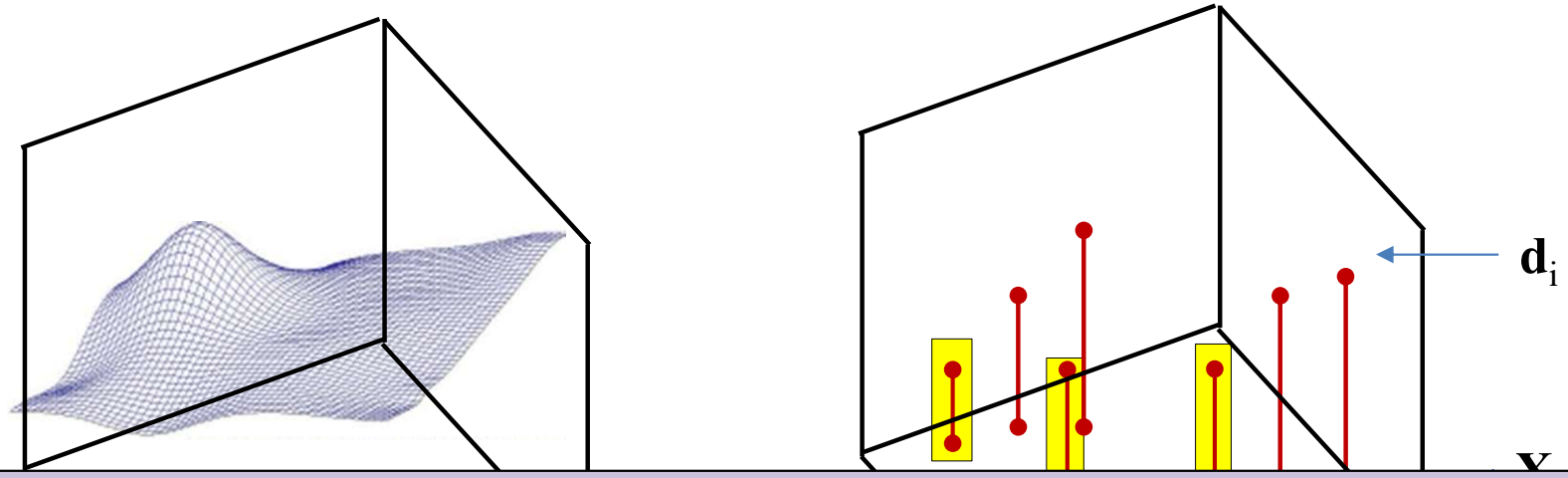
Mini Batches



The variance of the minibatch loss: var(BatchLoss) = 1/b var(div)
This will be much smaller than the variance of the sample error in SGD

The minibatch loss is also an unbiased estimate of the expected error

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- The *expected value* of the *batch loss* is also the *expected divergence*

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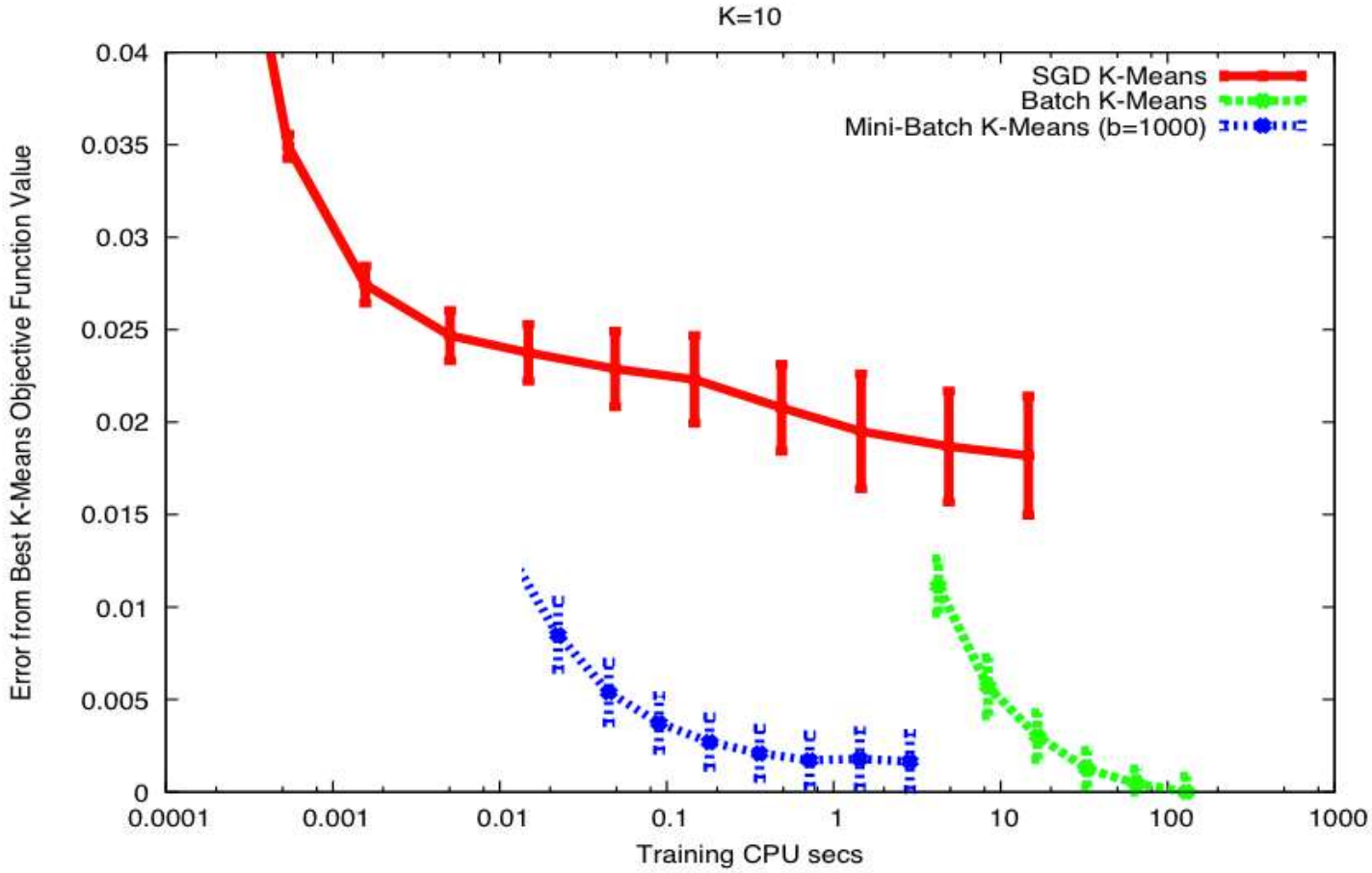
Minibatch convergence

- For convex functions, convergence rate for SGD is $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$.
- For *mini-batch* updates with batches of size b, the convergence rate is $\mathcal{O}\left(\frac{1}{\sqrt{bk}} + \frac{1}{k}\right)$
  - Apparently an improvement of $\sqrt{b}$ over SGD
  - But since the batch size is b, we perform b times as many computations per iteration as SGD
  - We actually get a *degradation* of $\sqrt{b}$
- However, in practice
  - The objectives are generally not convex; mini-batches are more effective with the right learning rates
  - We also get additional benefits of vector processing

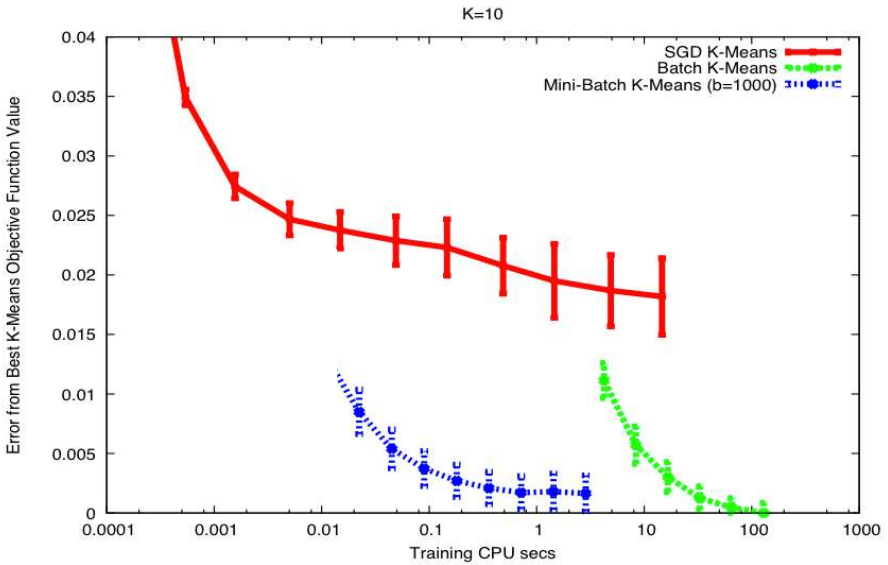
SGD example



- Mini-batch performs comparably to batch training on this simple problem
  - But converges orders of magnitude faster

Measuring Loss

- Convergence is generally defined in terms of the *overall training* loss
  - Not sample or batch loss



- Infeasible to actually measure the overall training loss after each iteration
- More typically, we estimate is as
  - Divergence or classification error on a held-out set
  - Average sample/batch loss over the past N samples/batches

Training and minibatches

- In practice, training is usually performed using mini-batches
  - The mini-batch size is generally set to the largest that your hardware will support (in memory) without compromising overall compute time
    - Larger minibatches = less variance
    - Larger minibatches = few updates per epoch
- Convergence depends on learning rate
  - Simple technique: fix learning rate until the error plateaus, then reduce learning rate by a fixed factor (e.g. 10)
  - ***Advanced methods***: Adaptive updates, where the learning rate is itself determined as part of the estimation

Poll 3

PIAZZA @531

Select all that are true

- Minibatch descent is an online version of batch updates
- Minibatch descent is faster than SGD when the batch size is 1
- The variance of minibatch updates decreases with batch size
- Minibatch gradient approaches batch updates in variance, but SGD in efficiency when we use vector processing and large batches

Poll 3

Select all that are true

- Minibatch descent is an online version of batch updates
- Minibatch descent is faster than SGD when the batch size is 1 **[false]**
- The variance of minibatch updates decreases with batch size
- Minibatch gradient approaches batch updates in variance, but SGD in efficiency when we use vector processing and large batches

Story so far

- SGD: Presenting training instances one-at-a-time can be more effective than full-batch training
  - Provided they are provided in random order
- For SGD to converge, the learning rate must shrink sufficiently rapidly with iterations
  - Otherwise the learning will continuously "chase" the latest sample
- SGD estimates have higher variance than batch estimates
- Minibatch updates operate on *batches* of instances at a time
  - Estimates have lower variance than SGD
  - Convergence rate is theoretically worse than SGD
  - But we compensate by being able to perform batch processing

Training and minibatches

- Convergence depends on learning rate
  - Simple technique: fix learning rate until the error plateaus, then reduce learning rate by a fixed factor (e.g. 10)
  - ***Advanced methods***: Adaptive updates, where the learning rate is itself determined as part of the estimation

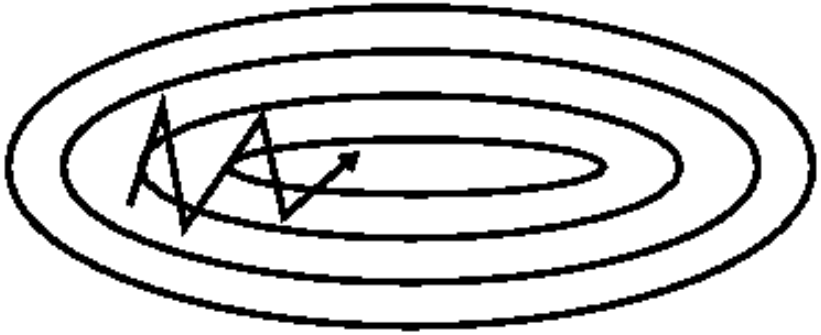
Moving on: Topics for the day

- Incremental updates
- Revisiting “trend” algorithms
- Generalization
- Tricks of the trade
  - Divergences..
  - Activations
  - Normalizations

Recall: Momentum Update

Plain gradient update

With momentum



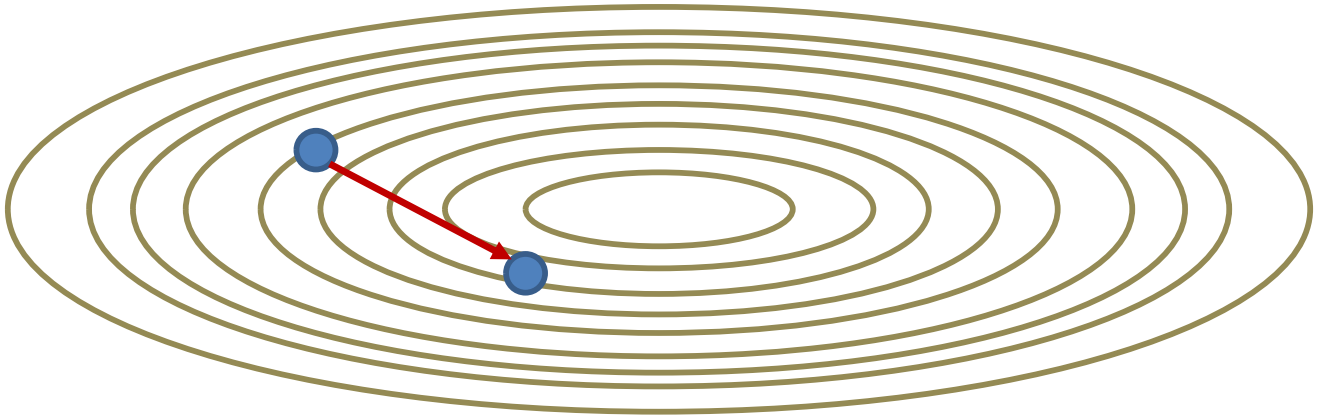
- The momentum method maintains a running average of all gradients until the *current* step

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^{\mathsf{T}}$$

$$W^{(k)} = W^{(k-1)} + \Delta W^{(k)}$$

  - Typical β value is 0.9
- The running average steps
  - Get longer in directions where gradient retains the same sign
  - Become shorter in directions where the sign keeps flipping

Recall: Momentum Update

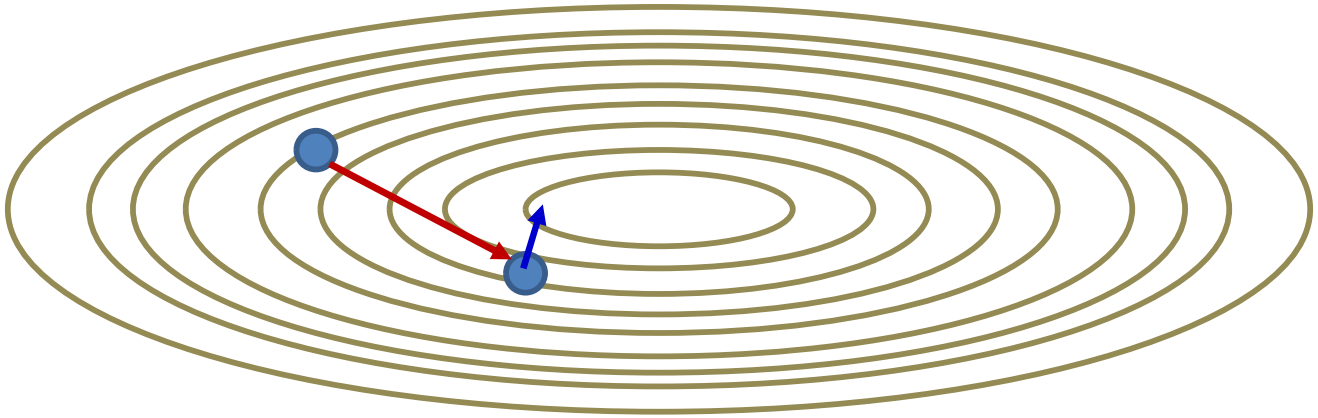


- The momentum method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

- At any iteration, to compute the current step:

Recall: Momentum Update

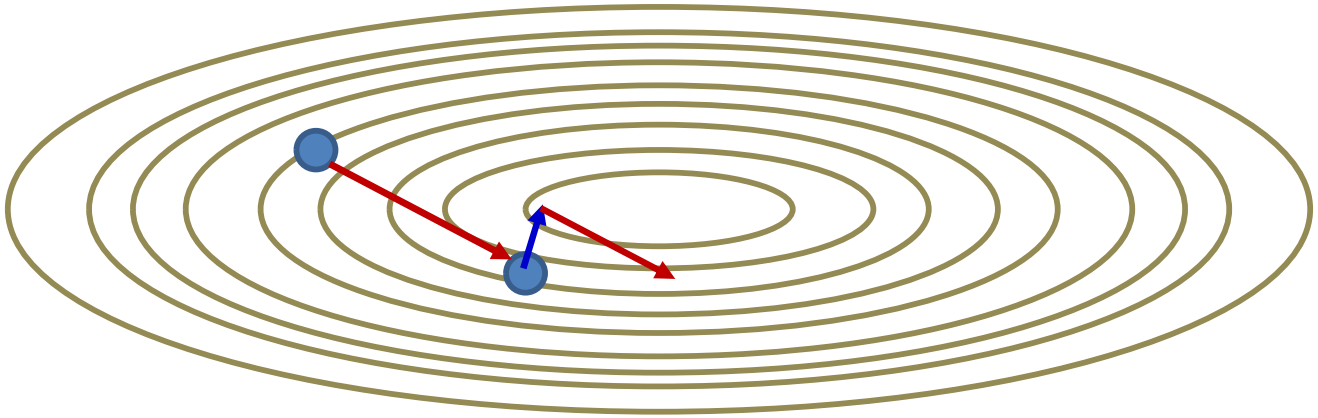


- The momentum method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

- At any iteration, to compute the current step:
  - First compute the gradient step at the current location

Recall: Momentum Update



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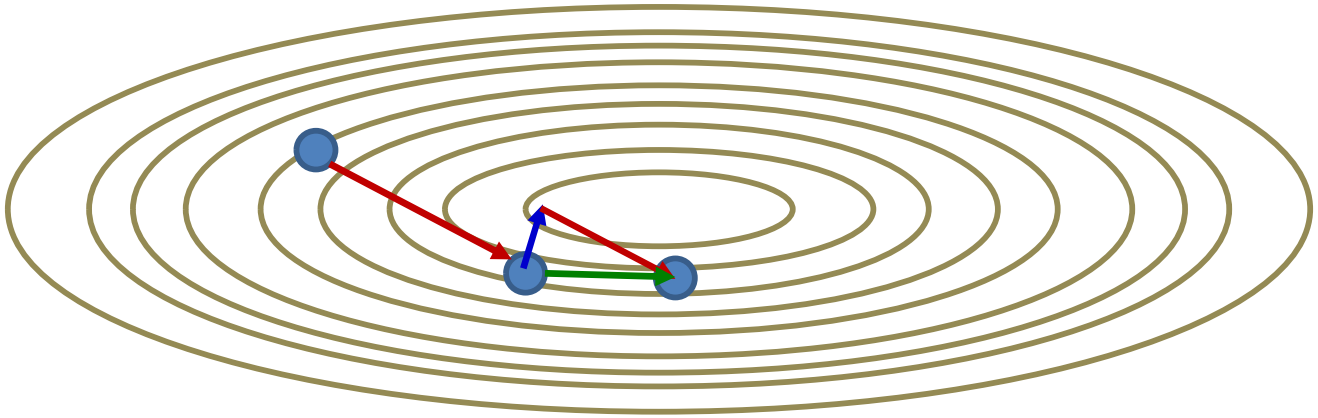
$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

- At any iteration, to compute the current step:
  - First compute the gradient step at the current location
  - Then add in the scaled *previous* step
    - Which is actually a running average

Recall: Momentum Update

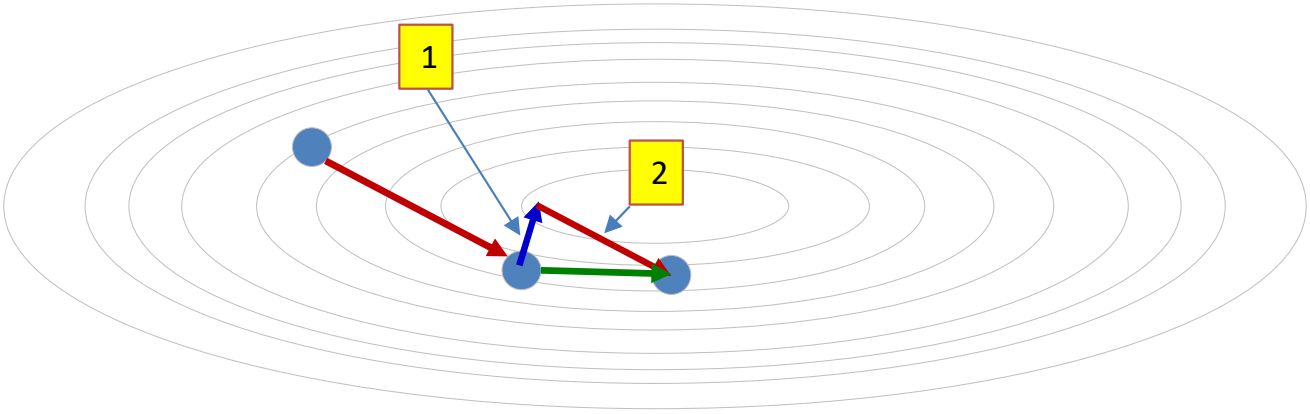


- The momentum method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

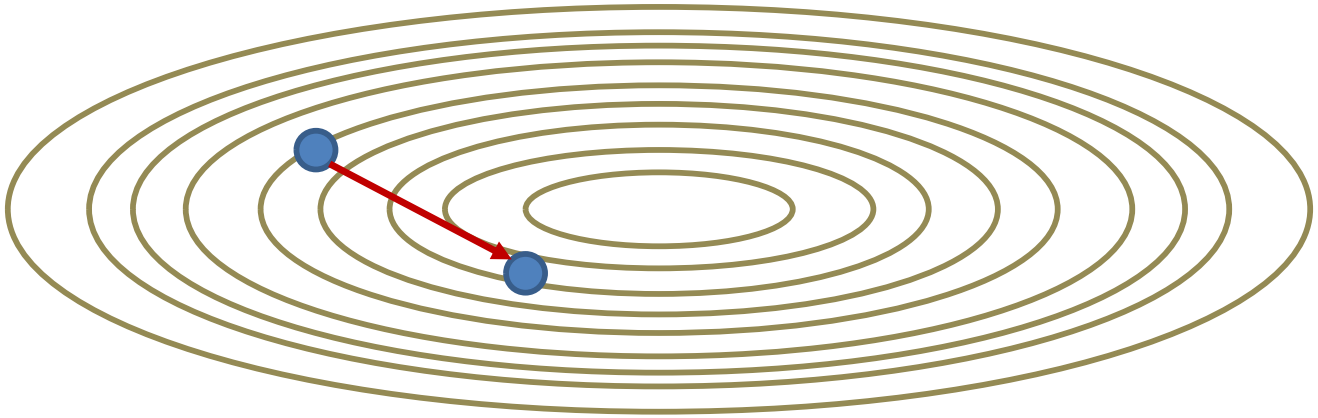
- At any iteration, to compute the current step:
  - First compute the gradient step at the current location
  - Then add in the scaled *previous* step
    - Which is actually a running average
  - To get the final step

Momentum update



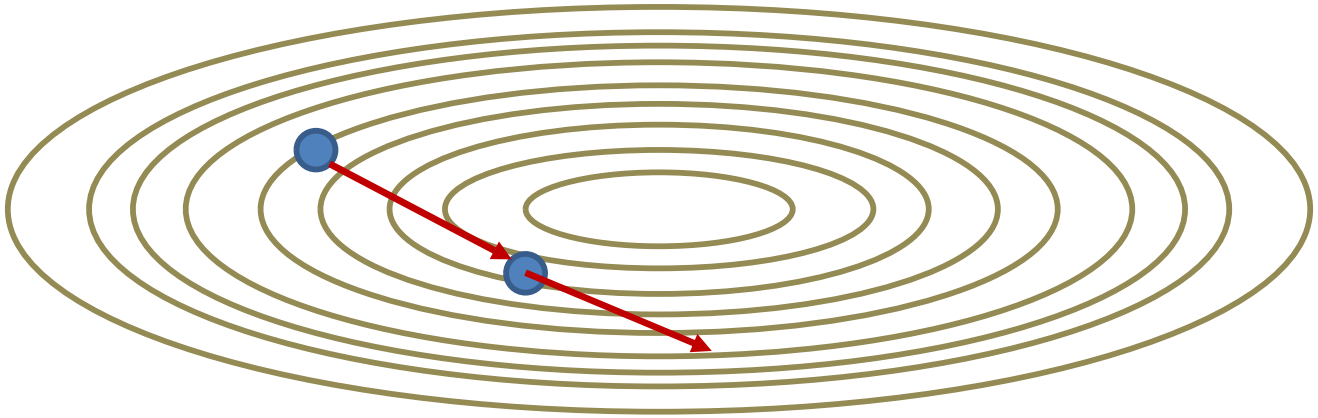
- Momentum update steps are actually computed in two stages
  - First: We take a step against the gradient at the current location
  - Second: Then we add a scaled version of the previous step
- The procedure can be made more optimal by reversing the order of operations..

Nestorov's Accelerated Gradient



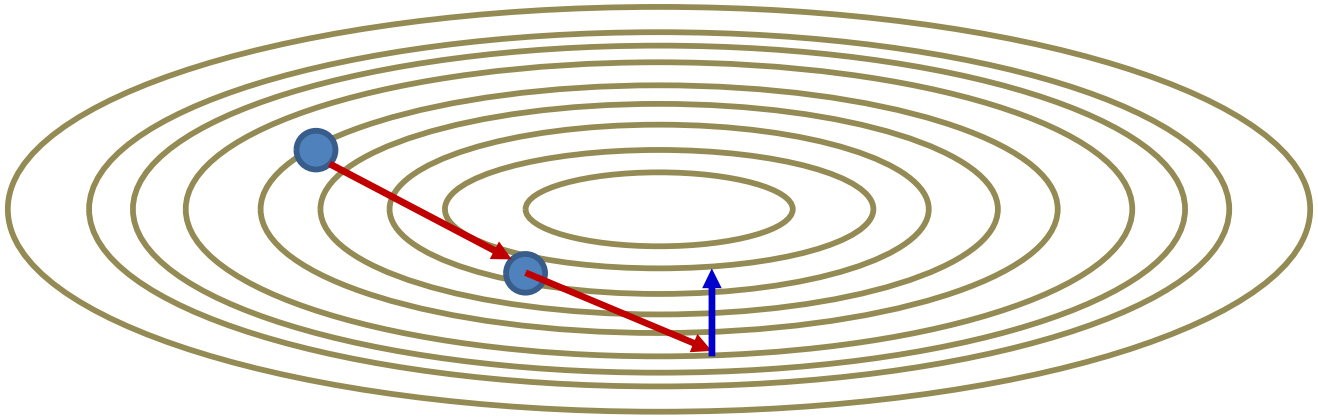
- Change the order of operations
- At any iteration, to compute the current step:

Nestorov's Accelerated Gradient



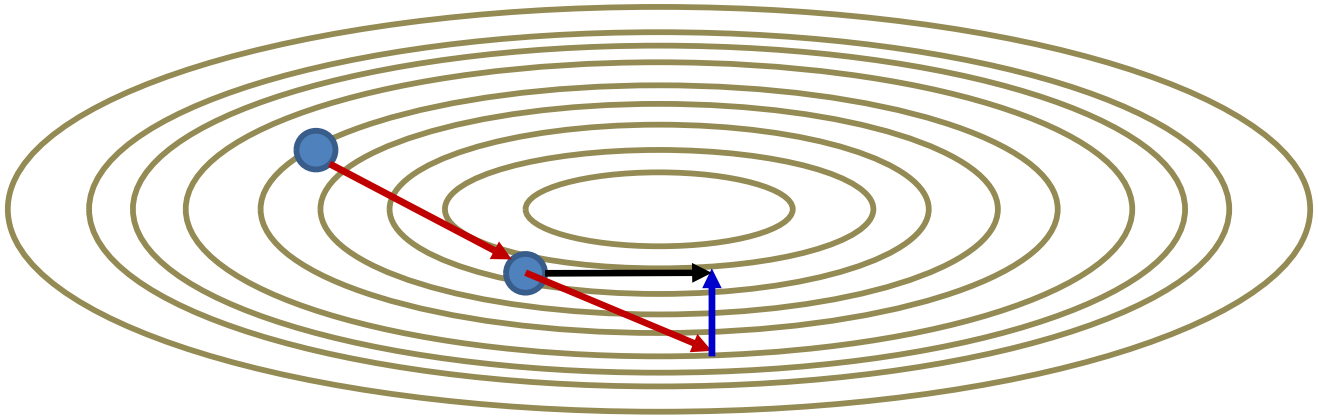
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step

Nestorov's Accelerated Gradient



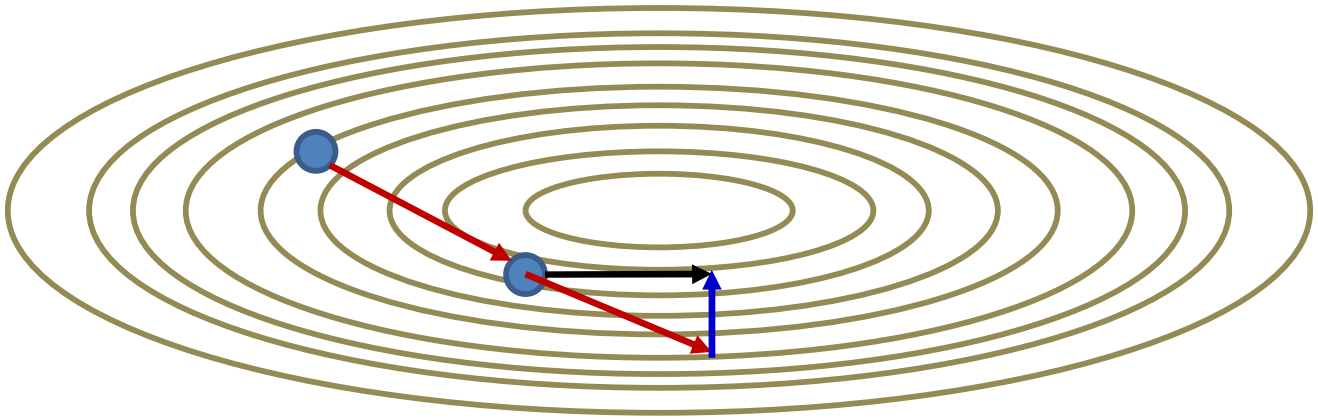
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step
  - Then compute the gradient step at the resultant position

Nestorov's Accelerated Gradient



- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step
  - Then compute the gradient step at the resultant position
  - Add the two to obtain the final step

Nestorov's Accelerated Gradient



- Nestorov's method

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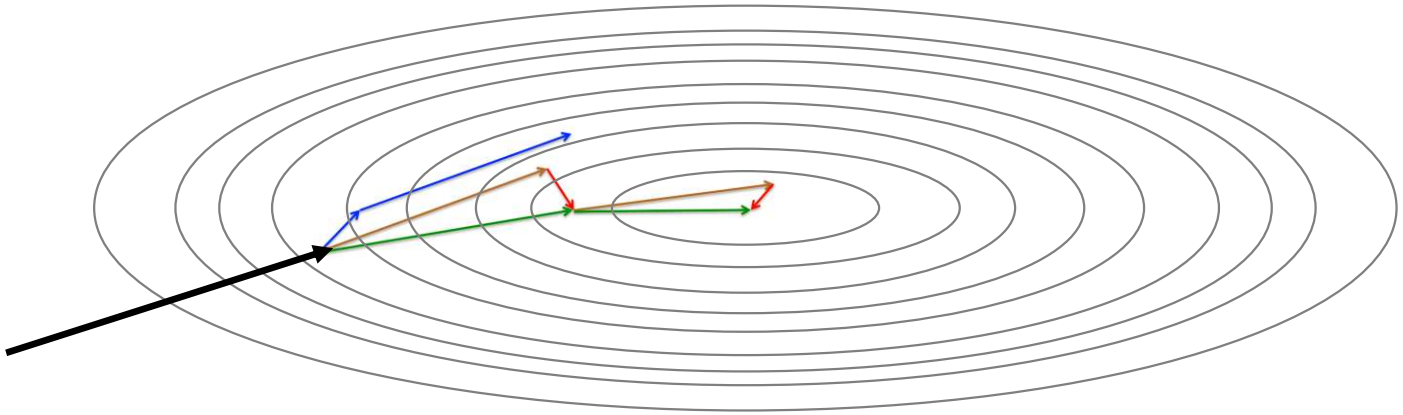
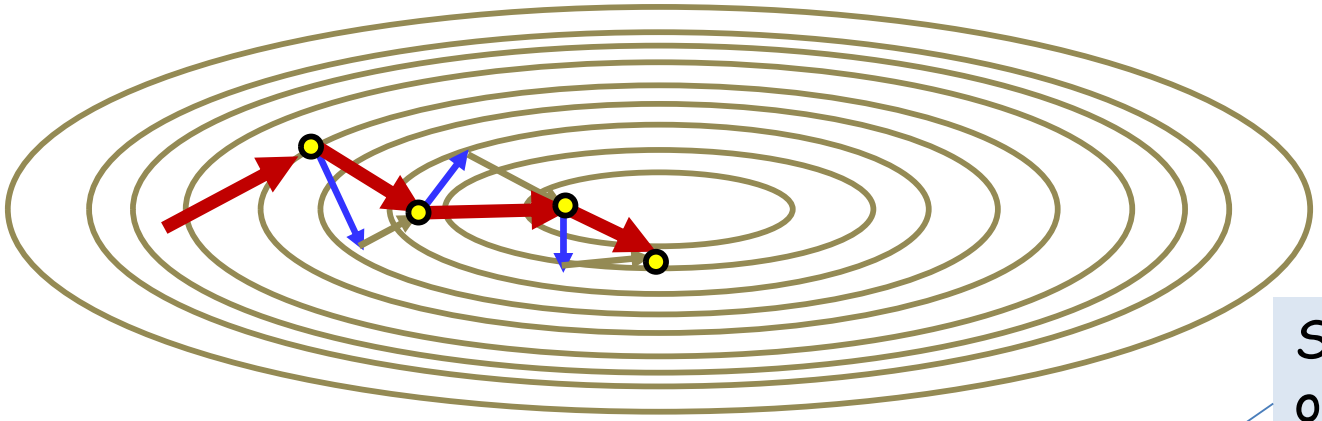
$$W^{(k)} = W^{(k-1)} + \Delta W^{(k)}$$

Nestorov's Accelerated Gradient



- Comparison with momentum (example from Hinton)
- Converges much faster

Momentum and incremental updates



SGD instance or minibatch loss

- The momentum method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

- Incremental SGD and mini-batch gradients tend to have high variance
- Momentum smooths out the variations
  - Smoother and faster convergence

Momentum: Mini-batch update

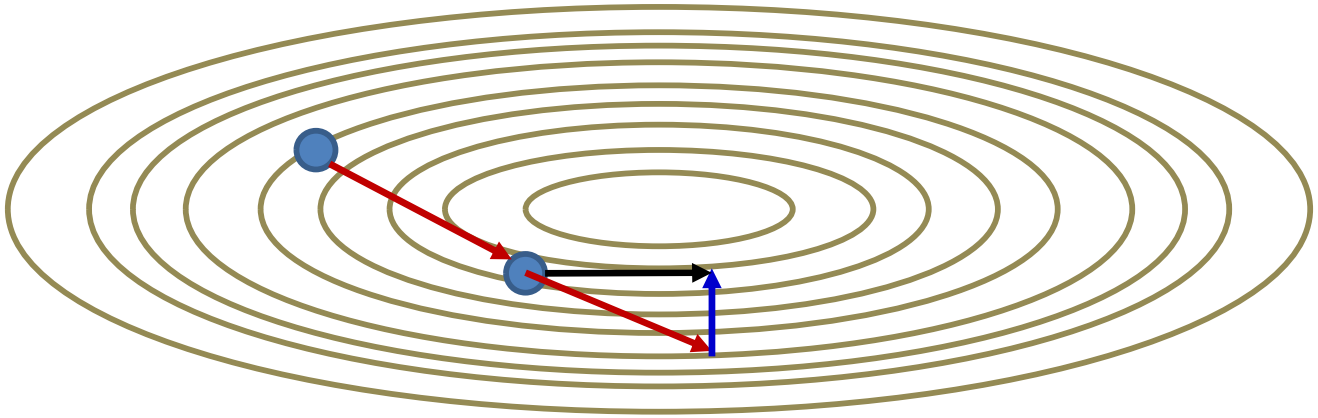
- Given (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$, $\Delta W_k = 0$
- Do:
  - Randomly permute (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
  - For $t = 1 : b : T$
    - $j = j + 1$
    - For every layer k:
      - $\nabla_{W_k} Loss = 0$
    - For t' = t : t+b-1
      - For every layer k:
        - » Compute $\nabla_{W_k} Div(Y_t, d_t)$
        - » $\nabla_{W_k} Loss \mathrel{+}= \frac{1}{b} \nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
    - Update
      - For every layer k:

$$\Delta W_k = \beta \Delta W_k - \eta_j (\nabla_{W_k} Loss)^T$$

$$W_k = W_k + \Delta W_k$$

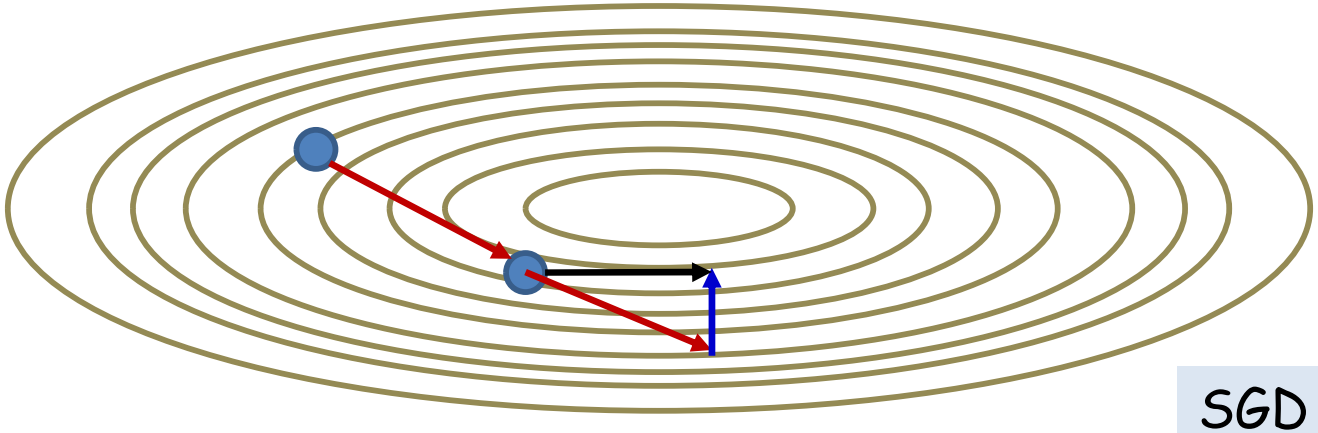
- Until $Loss$ has converged

Nestorov's Accelerated Gradient



- At any iteration, to compute the current step:
  - First extend the previous step
  - Then compute the gradient at the resultant position
  - Add the two to obtain the final step
- This also applies directly to incremental update methods
  - The accelerated gradient smooths out the variance in the gradients

Nestorov's Accelerated Gradient



SGD instance or minibatch loss

- Nestorov's method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss(W^{(k-1)} + \beta \Delta W^{(k-1)})^T$$

$$W^{(k)} = W^{(k-1)} + \Delta W^{(k)}$$

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        - $\nabla_{W_k} Loss \mathrel{+}= \frac{1}{b} \nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
    - Update
      - For every layer k:

$$W_k = W_k - \eta_j \nabla_{W_k} Loss^T$$
$$\Delta W_k = \beta \Delta W_k - \eta_j \nabla_{W_k} Loss^T$$

- Until $Loss$ has converged

The other term in the update

- Standard gradient descent rule

$$W \leftarrow W - \eta \nabla_W L(W)$$

- Gradient descent invokes two terms for updates
  - The derivative
  - and the learning rate

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- Standard gradient descent rule

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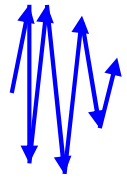
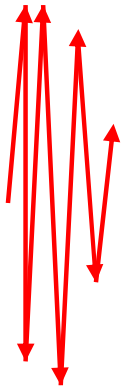
- Gradient descent invokes two terms for updates
  - The derivative
  - and the learning rate
- Momentum methods fix this term to reduce unstable oscillation
- What about this term?

Adjusting the learning rate

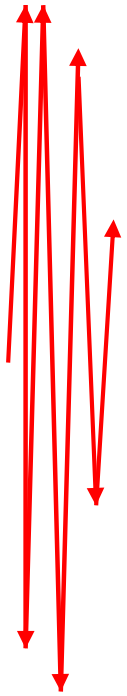
Sequence of gradients



vs



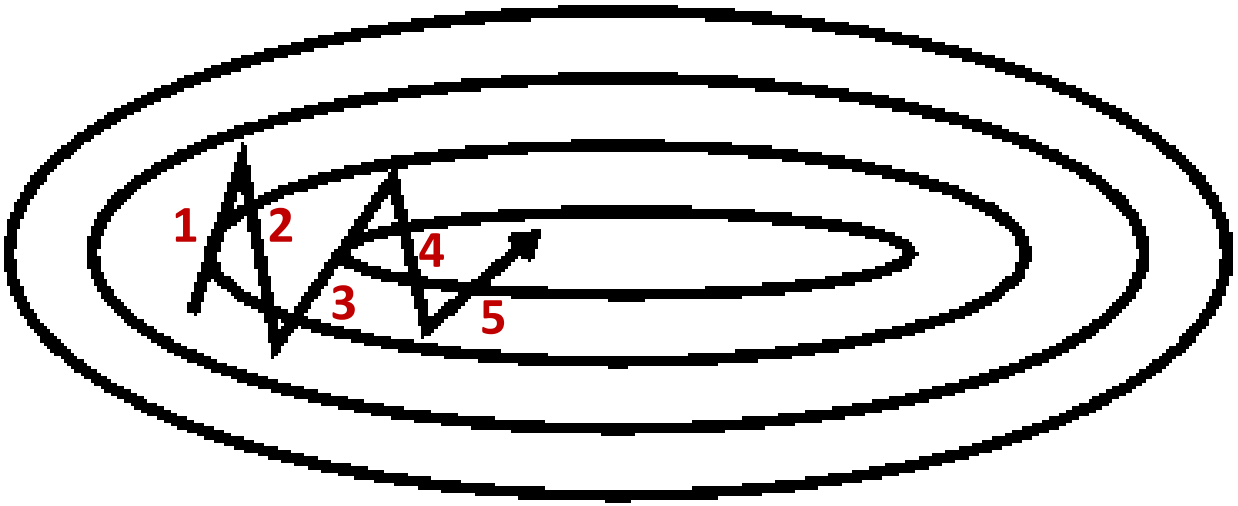
vs



With separate learning rates in each direction, which should have the lowest learning rate in the vertical direction?

- Have separate learning rates for each component
- Directions in which the derivatives swing more should likely have lower learning rates
  - Is likely indicative of more wildly swinging behavior
- Directions of greater swing are indicated by total movement
  - Direction of greater movement should have lower learning rate

Smoothing the trajectory



Step	X component	Y component
1	1	+2.5
2	1	-3
3	2	+2.5
4	1	-2
5	1.5	1.5

- Observation: Steps in "oscillatory" directions show large total movement
  - In the example, total motion in the vertical direction is much greater than in the horizontal direction
- Solution: Lower learning rate in the vertical direction than in the horizontal direction
  - Based on total motion
  - As quantified by RMS value

RMS Prop

- Notation:
  - Formulae are ***by parameter***
  - Derivative of loss w.r.t any individual parameter w is shown as $\partial_w D$
    - Batch or minibatch loss, or individual divergence for batch/minibatch/SGD
  - The ***squared*** derivative is $\partial_w^2 D = (\partial_w D)^2$
    - Short-hand notation represents the squared derivative, not the second derivative
  - The ***mean squared*** derivative is a running estimate of the average squared derivative. We will show this as $E[\partial_w^2 D]$
- Modified update rule: We want to
  - scale down learning rates for terms with large mean squared derivatives
  - scale up learning rates for terms with small mean squared derivatives

RMS Prop

- This is a variant on the *basic* mini-batch SGD algorithm

- **Procedure:**
  - Maintain a running estimate of the mean squared value of derivatives for each parameter
  - Scale learning rate of the parameter by the *inverse* of the *root mean squared* derivative

$$E[\partial_w^2 D]_k = \gamma E[\partial_w^2 D]_{k-1} + (1-\gamma)(\partial_w^2 D)_k$$

$$w_{k+1} = w_k - \frac{\eta}{\sqrt{E[\partial_w^2 D]_k + \epsilon}} \partial_w D$$

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Note similarity to RPROP
The magnitude of the derivative is being normalized out

RMS Prop (updates are for each weight of each layer)

- Do:
  - Randomly shuffle inputs to change their order
  - Initialize: $k = 1$; for all weights w in all layers, $E[\partial_w^2 D]_k = 0$
  - For all $t = 1:B:T$ (incrementing in blocks of B inputs)
    - For all weights in all layers initialize $(\partial_w D)_k = 0$
    - For $b = 0:B-1$
      - Compute
        - » Output $\boldsymbol{Y(X_{t+b})}$
        - » Compute gradient $\frac{\boldsymbol{dDiv(Y(X_{t+b}),d_{t+b})}}{\boldsymbol{dw}}$
        - » Compute $(\partial_w D)_k \mathrel{+}= \frac{1}{B}\frac{\boldsymbol{dDiv(Y(X_{t+b}),d_{t+b})}}{\boldsymbol{dw}}$
    - update: for all $w \in \{w_{\{ij\}}^k \forall i,j,k\}$

$$\boldsymbol{E[\partial_w^2 D]_k = \gamma E[\partial_w^2 D]_{k-1} + (1-\gamma)(\partial_w^2 D)_k}$$

$$\boldsymbol{w_{k+1} = w_k - \frac{\eta}{\sqrt{E[\partial_w^2 D]_k + \epsilon}}\partial_w D}$$

    - $k = k + 1$
- Until loss has converged

Typical values:
$\gamma = 0.9$
$\eta = 0.001$

All the terms in gradient descent

- Standard gradient descent rule

$$W \leftarrow W - \eta \nabla_W L(W)$$

- RMSprop only adapts the learning rate
  - by total movement
- Momentum only smooths the gradient

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- How about combining both?

ADAM: RMSprop with momentum

- RMS prop only adapts the learning rate
- Momentum only smooths the gradient
- ADAM combines the two

- **Procedure:**
  - Maintain a running estimate of the mean derivative for each parameter
  - Maintain a running estimate of the mean squared value of derivatives for each parameter
  - Scale update of the parameter by the *inverse* of the *root mean squared* derivative

$$m_k = \delta m_{k-1} + (1-\delta)(\partial_w D\,)_k$$

$$v_k = \gamma v_{k-1} + (1-\gamma)(\partial_w^2 D)_k$$

$$\hat{m}_k = \frac{m_k}{1-\delta^k}, \qquad \hat{v}_k = \frac{v_k}{1-\gamma^k}$$

$$w_{k+1} = w_k - \frac{\eta}{\sqrt{\hat{v}_k + \epsilon}}\hat{m}_k$$

ADAM: RMSprop with momentum

- RMS prop only adapts the learning rate
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- **Procedure:**
  - Maintain a running estimate of the mean derivative for each parameter
  - Maintain a running estimate of the mean squared valu parameter
  - Scale update of the parameter by the *inverse* of the derivative

Ensures that the δ and γ terms do not dominate in early iterations

$$m_k = \delta m_{k-1} + (1-\delta)(\partial_w D)_k$$

$$v_k = \gamma v_{k-1} + (1-\gamma)(\partial_w^2 D)_k$$

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ADAM: RMSprop with momentum

Typically μ_0 is 0 and δ is close to 1. So $(1-\delta) \approx 0$.
Without the denominator term μ_k will stay close to 0 for $k = 0,1,2, \ldots$ for a long time, resulting in minimal parameter updates

The denominator term ensures that $\mu_1 = (\partial_w D)_1$ and updates actually happen

For large k, the denominator just becomes 1

- Maintain a running estimate of the mean squared valu… parameter
- Scale update of the parameter by the *inverse* of the… derivative

Ensures that the δ and γ terms do not dominate in early iterations

$$m_k = \delta m_{k-1} + (1-\delta)(\partial_w D)_k$$

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$$\hat{m}_k = \frac{m_k}{1-\delta^k}, \qquad \hat{v}_k = \frac{v_k}{1-\gamma^k}$$

$$w_{k+1} = w_k - \frac{\eta}{\sqrt{\hat{v}_k + \epsilon}} \hat{m}_k$$

Other variants of the same theme

- Many:
  - Adagrad
  - AdaDelta
  - AdaMax
  - …
- Generally no explicit learning rate to optimize
  - But come with other hyper parameters to be optimized
  - Typical params:
    - RMSProp: $\eta = 0.001, \gamma = 0.9$
    - ADAM: $\eta = 0.001, \delta = 0.9, \gamma = 0.999$

Poll 4

PIAZZA @532

Which of the following are true

- Vanilla SGD considers the long-term trends of gradients in update steps
- Momentum methods consider the long-term average of derivatives to make updates
- RMSprop only considers the second order moment of derivatives, but not their average trend, to make updates
- ADAM considers both the average trend and second moment of derivatives to make updates
- Trend-based optimizers like momentum, RMSprop and ADAM are important to smooth out the variance of SGD or minibatch updates

Poll 4

Which of the following are true

- Vanilla SGD considers the long-term trends of gradients in update steps **[false]**
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- RMSprop only considers the second order moment of derivatives, but not their average trend, to make updates
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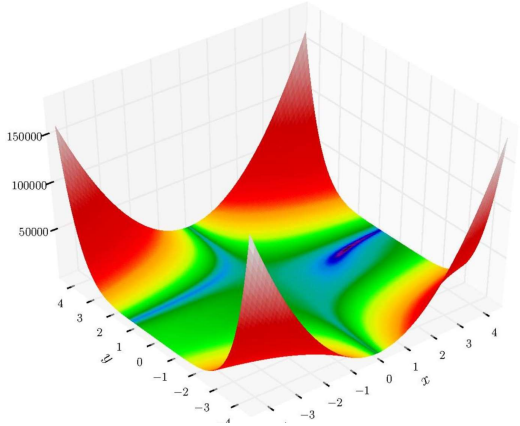
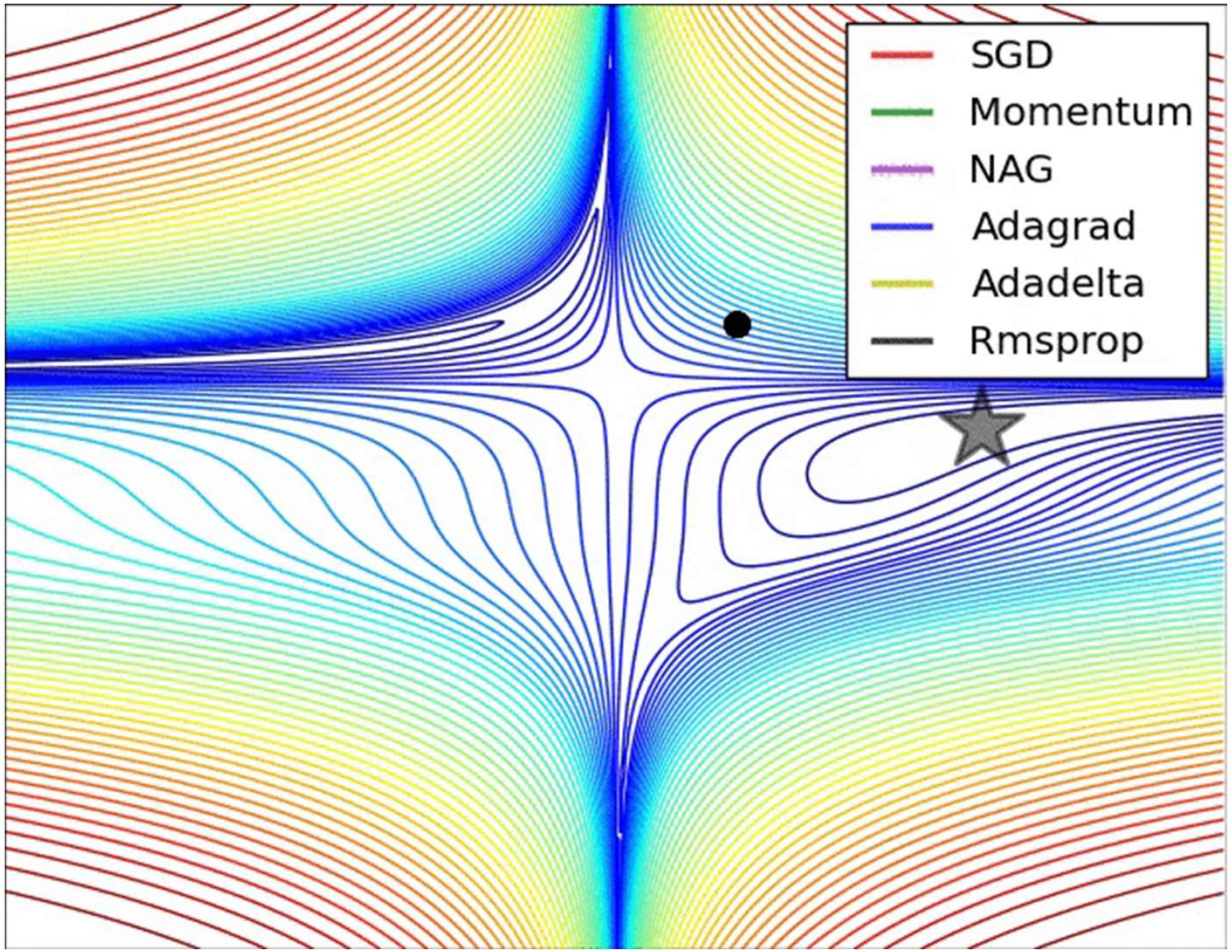
- Trend-based optimizers like momentum, RMSprop and ADAM are important to smooth out the variance of SGD or minibatch updates

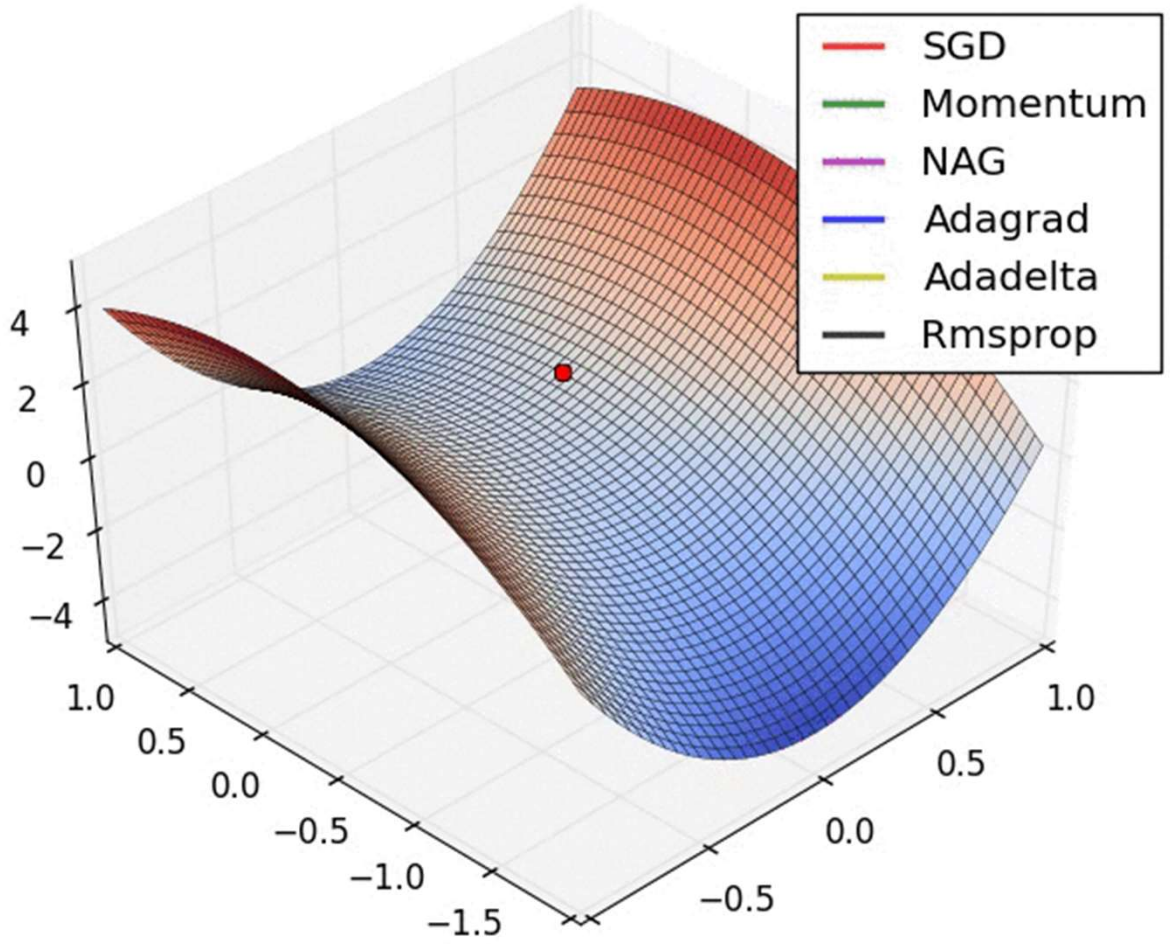
Visualizing the optimizers: Beale's Function





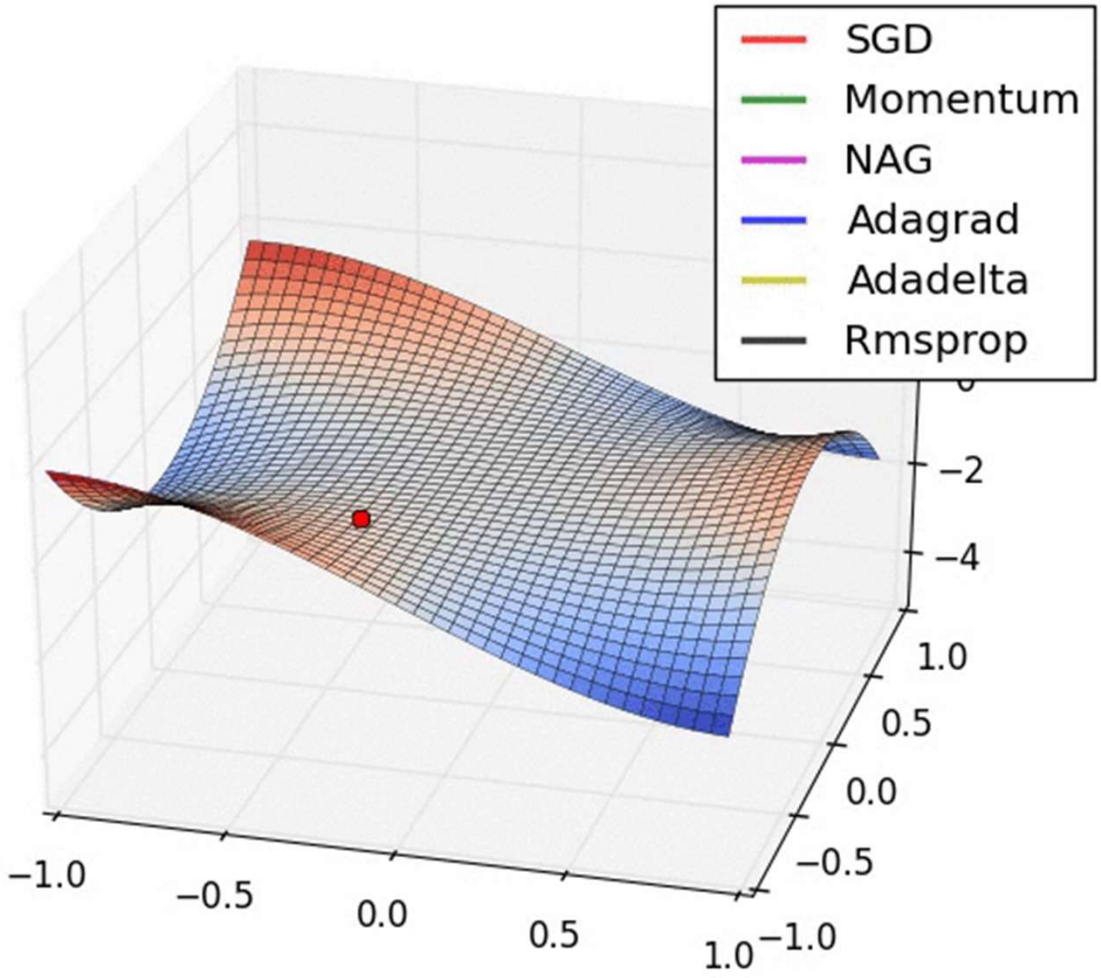
- http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

Visualizing the optimizers: Long Valley



- http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

Visualizing the optimizers: Saddle Point



- http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

Story so far

- Gradient descent can be sped up by incremental updates
  - Convergence is guaranteed under most conditions
    - Learning rate must shrink with time for convergence
  - Stochastic gradient descent: update after each observation. Can be much faster than batch learning
  - Mini-batch updates: update after batches. Can be more efficient than SGD

- Convergence can be improved using smoothed updates
  - RMSprop and more advanced techniques