Training Neural Networks: Optimization

Intro to Deep Learning, Fall 2020

Quick Recap

- Gradient descent, Backprop

Quick Recap: Training a network

Total loss

Average over all training instances

Divergence between desired output and actual output of net for a given input X

Output of net in response to input X

Desired output in response to input X

$$L(W) = \frac{1}{N_X} \sum_X div(f(X;W), D(X))$$

$$\boxed{\widehat{W} = \underset{W}{\arg\min}\, L(W)}$$

- Define a total "loss" over all training instances
  - Quantifies the difference between desired output and the actual output, as a function of weights
- Find the weights that minimize the loss

Quick Recap: Training networks by gradient descent

$$L(W) = \frac{1}{N_X} \sum_X div(f(X; W), D(X))$$

$$\nabla_W L(W) = \frac{1}{N_X} \sum_X \nabla_W div(f(X; W), D(X))$$

$$\boxed{\widehat{W} = \underset{W}{\arg\min}\, L(W)} \xrightarrow{\text{Solved through gradient descent as}} \boxed{W_k = W_{k-1} - \eta \nabla_W L(W)^T}$$

- The gradient of the total loss is the average of the gradients of the loss for the individual instances
- The total gradient can be plugged into gradient descent update to learn the network

Quick Recap: Training networks by gradient descent

$$L(W) = \frac{1}{N_X}\sum_X d$$

$$\nabla_W L(W) = \frac{1}{N_X}\sum_X \overbrace{\nabla_W div(f(X;W), D(X))}^{\text{Computed using backpropagation}}$$

Solved through gradient descent as

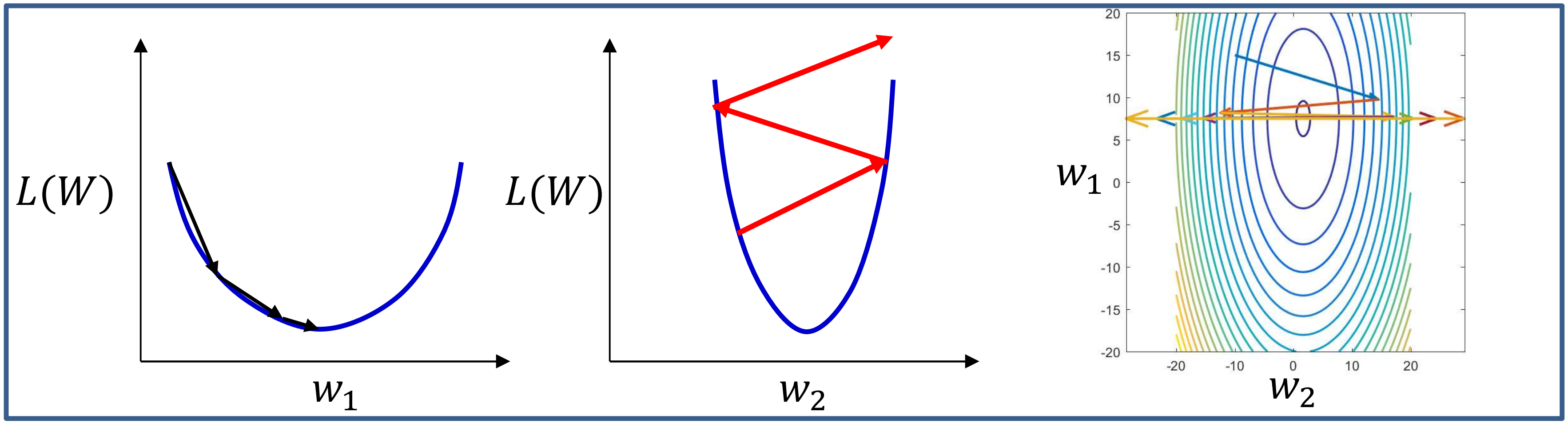
$$\boxed{\widehat{W} = \arg\min_W L(W)} \Rightarrow \boxed{W_k = W_{k-1} - \eta \nabla_W L(W)^T}$$

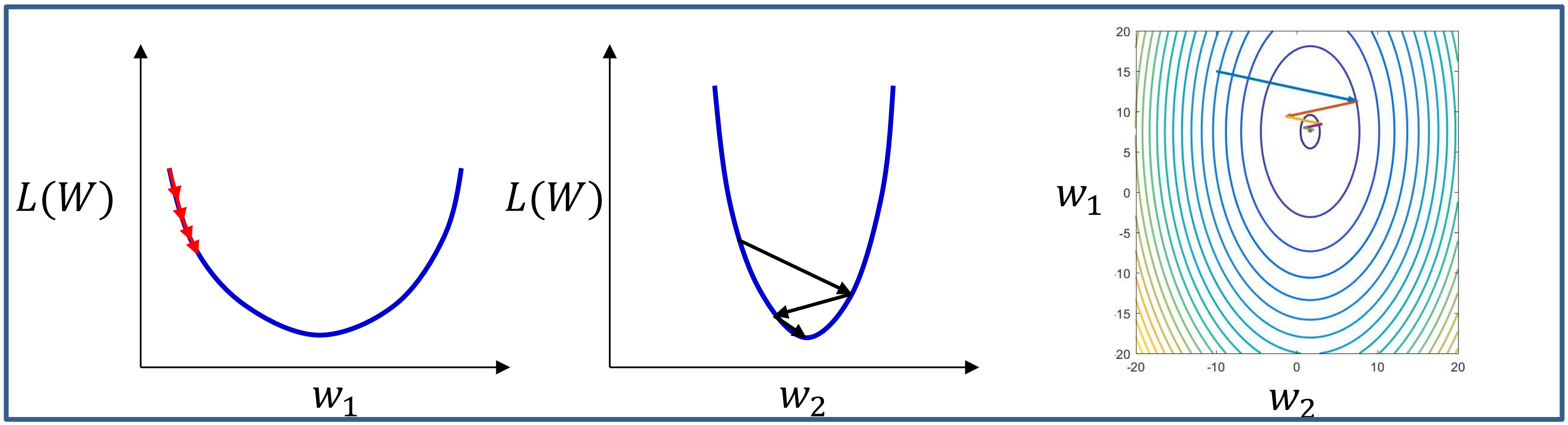
- The gradient of the total loss is the average of the gradients of the loss for the individual instances
- The gradient can be plugged into gradient descent update to learn the network parameters

Quick Recap

- Gradient descent, Backprop
- The issues with backprop and gradient descent
  - 1. Minimizes a *loss* which *relates* to classification accuracy, but is not actually classification accuracy
    - The divergence is a continuous valued proxy to classification error
    - Minimizing the loss is *expected* to, but not *guaranteed* to minimize classification error
  - 2. Simply minimizing the loss is hard enough..

Quick recap: Problem with gradient descent

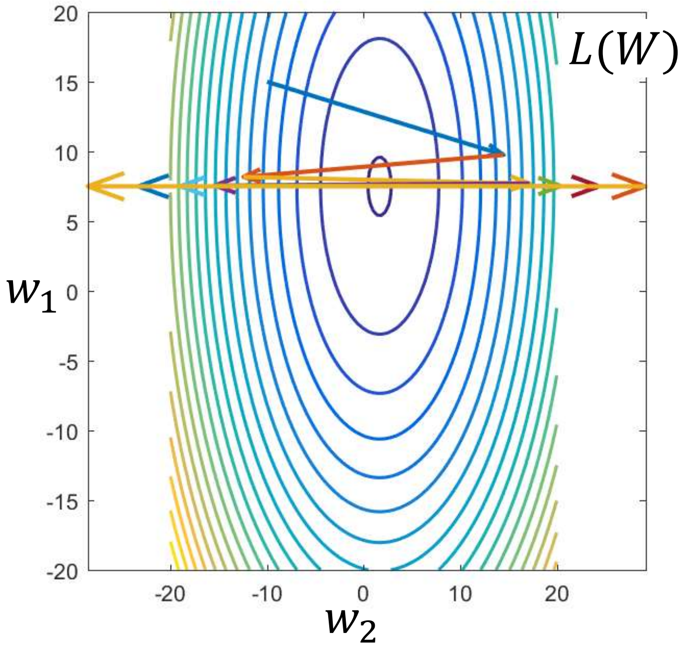


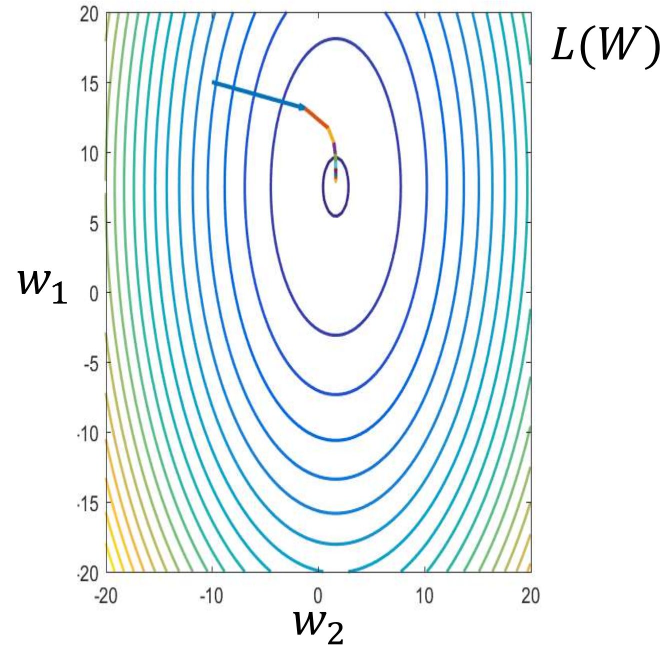


$$\boxed{W_k = W_{k-1} - \eta \nabla_w L(W)^T}$$

- A step size that assures fast convergence for a given eccentricity can result in divergence at a higher eccentricity
- .. Or result in extremely slow convergence at lower eccentricity

Quick recap: Problem with gradient descent



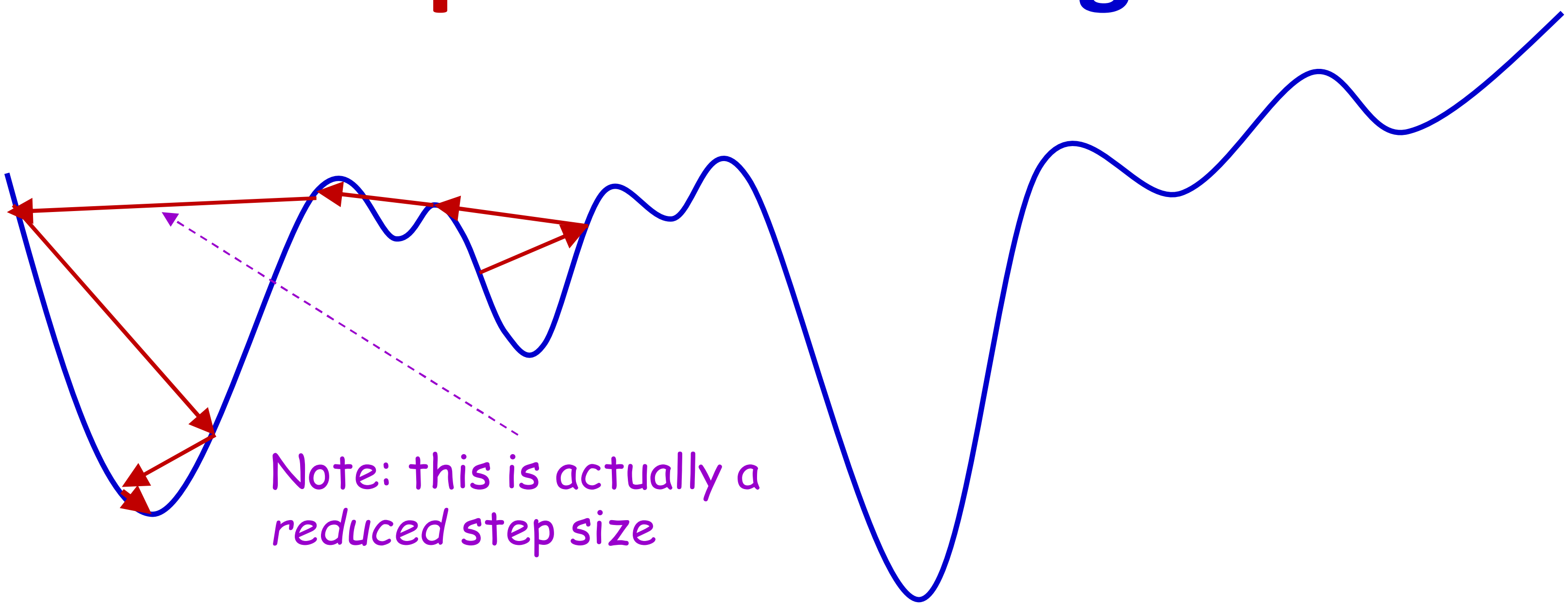


- The loss is a function of many weights (and biases)
  - Has different eccentricities w.r.t different weights
- A fixed step size for all weights in the network can result in the convergence of one weight, while causing a divergence of another

Story so far : Second-order methods

- Second-order methods “normalize” the variation along the components to mitigate the problem of different optimal learning rates for different components
  - But this requires computation of inverses of second-order derivative matrices
  - Computationally infeasible
  - Not stable in non-convex regions of the loss surface
  - Approximate methods address these issues, but simpler solutions may be better

Recap: The learning rate



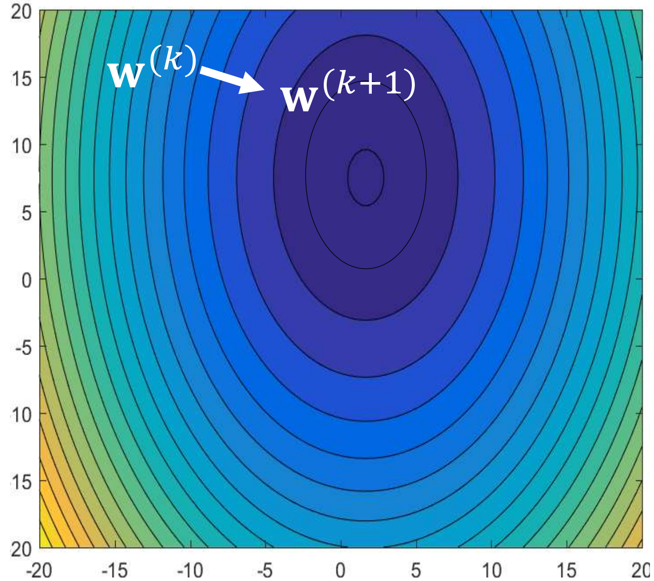
- For complex models such as neural networks the loss function is often not convex
  - Having $\eta > 2\eta_{opt}$ can actually help escape local optima
- Better to start with a large (divergent) learning rate and slowly shrink it over iterations
  - More likely to find better minima

Story so far : Learning rate

- Divergence-causing learning rates may not be a bad thing
  – Particularly for ugly loss functions
- *Decaying* learning rates provide good compromise between escaping poor local minima and convergence

- *Many of the convergence issues arise because we force the same learning rate on all parameters*

Lets take a step back



$$\boxed{\mathbf{w}^{(k+1)} \leftarrow \mathbf{w}^{(k)} - \eta(\nabla_{\mathbf{w}} E)^T}$$

$$\boxed{w_i^{(k+1)} = w_i^{(k)} - \eta \frac{dE\left(w_i^{(k)}\right)}{dw}}$$

- Problems arise because of requiring a fixed step size across all dimensions
  – Because step are “tied” to the gradient
- Let’s try releasing this requirement

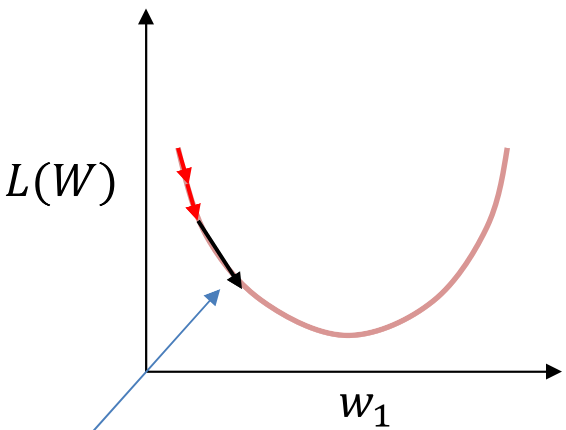
Story so far

- Gradient descent can miss obvious answers
  - And this may be a *good* thing
- Vanilla gradient descent may be too slow or unstable due to the differences between the dimensions
- Second order methods can normalize the variation across dimensions, but are complex
- Adaptive or decaying learning rates can improve convergence
- Methods that decouple the dimensions can improve convergence
- Momentum methods which emphasize directions of steady improvement are demonstrably superior to other methods

Quick Summary

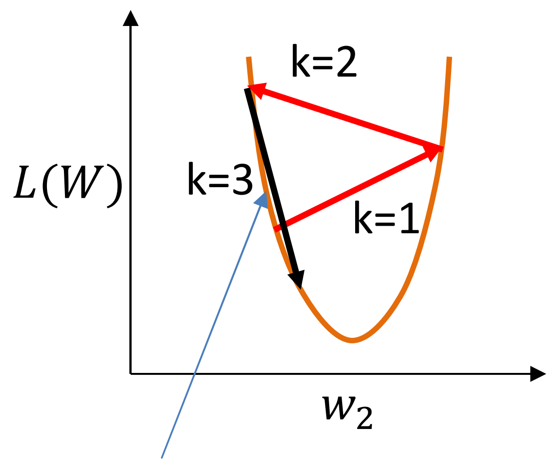
- Gradient descent, Backprop
- The issues with backprop and gradient descent
- Momentum methods..

Momentum methods: principle

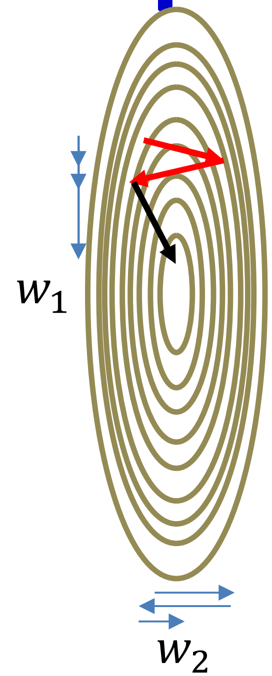


Increase stepsize because previous updates consistently moved weight right

$$\boxed{W_k = W_{k-1} - \eta \nabla_w L(W)^T}$$



Decrease stepsize because previous updates kept changing direction

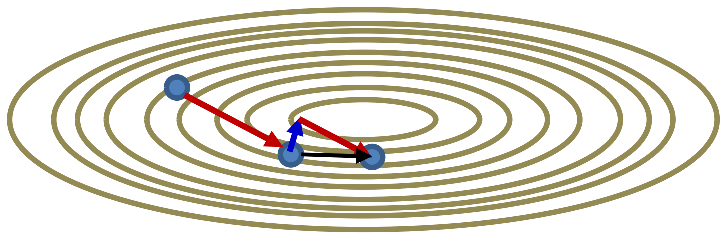


Stepsize shrinks along w2 but increases along w1

- Ideally: Have component-specific step size
  - But the resulting updates will not be against the gradient and do not guarantee descent
- Adaptive solution: Start with a common step size
  - *Shrink* step size in directions where the weight oscillates
  - *Expand* step size in directions where the weight moves consistently in one direction

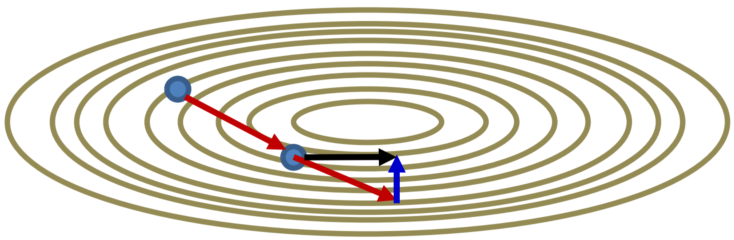
Quick recap: Momentum methods

Momentum



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

Nestorov



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

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

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

- Momentum: Retain gradient value, but *smooth out* gradients by maintaining a running average
  - Cancels out steps in directions where the weight value oscillates
  - Adaptively increases step size in directions of consistent change

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

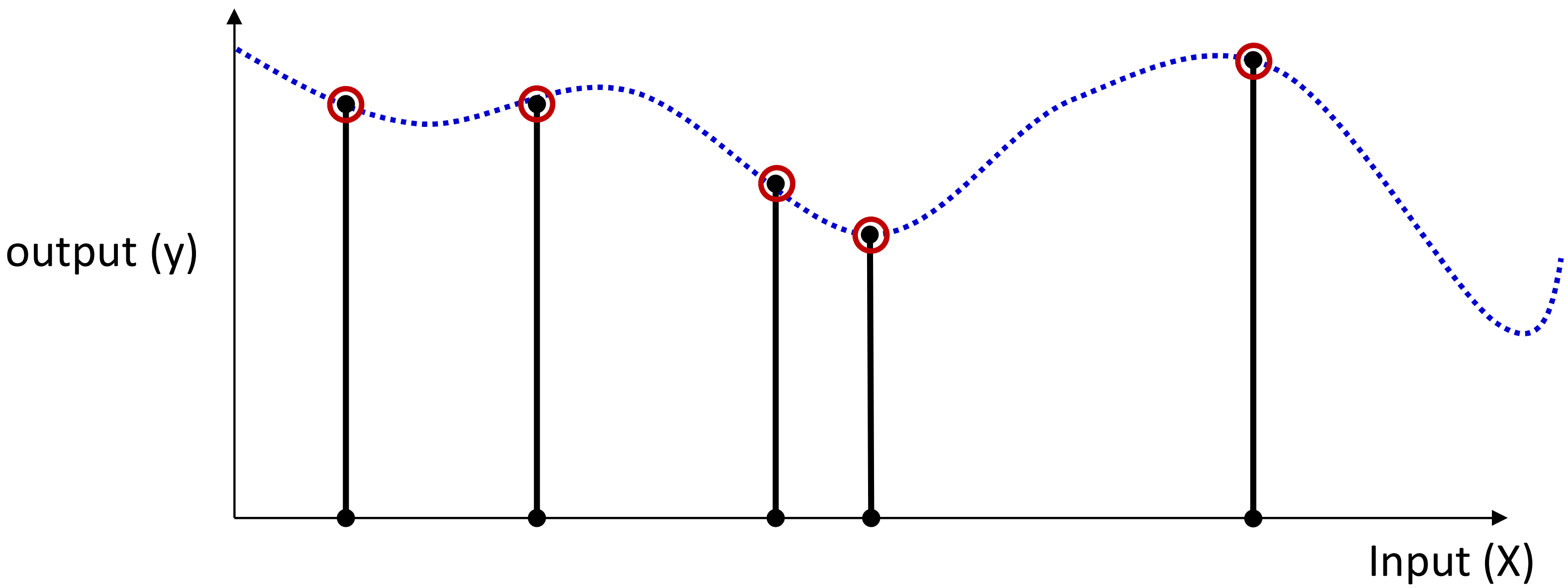
Moving on…

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

Moving on: Topics for the day

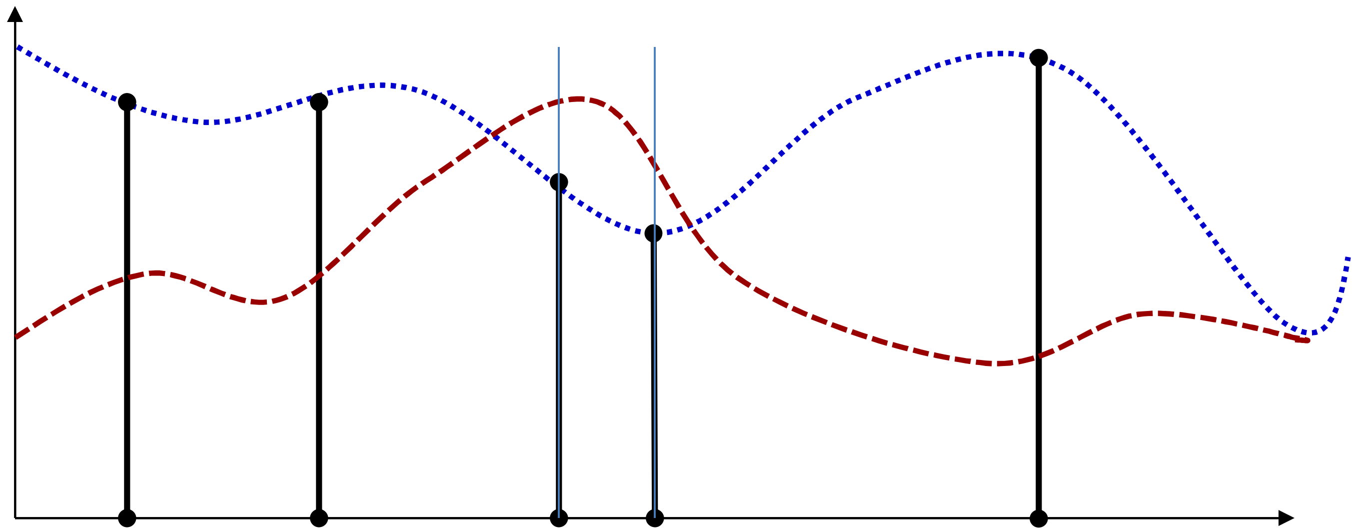
- Incremental updates
- Revisiting “trend” algorithms
- Generalization
- Tricks of the trade
  - Divergences..
  - Activations
  - Normalizations

The training formulation



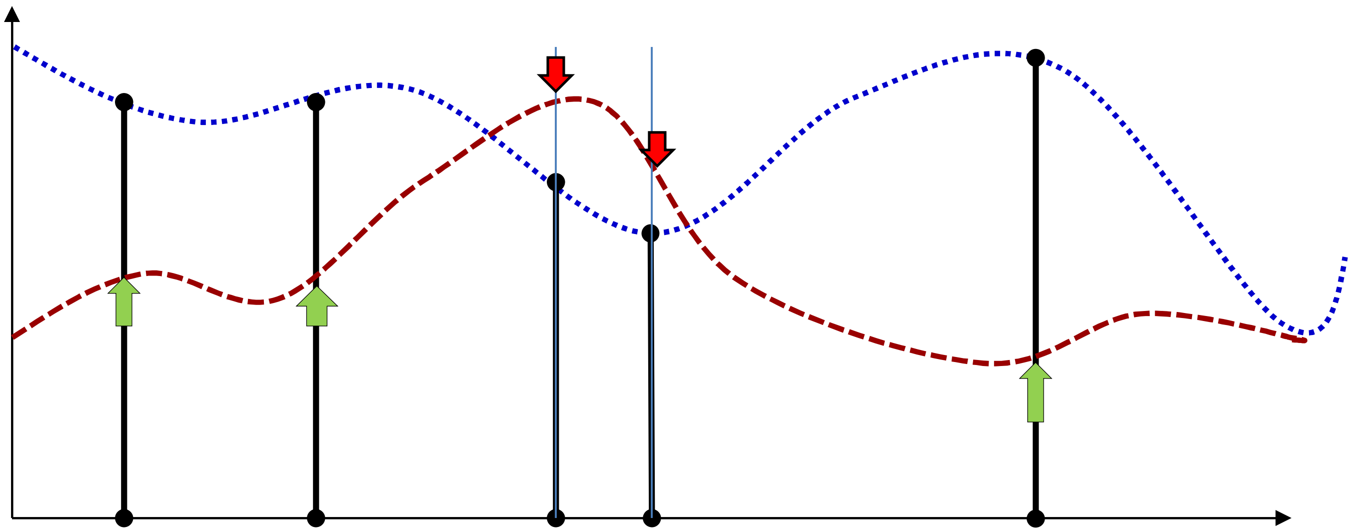
- Given input output pairs at a number of locations, estimate the entire function

Gradient descent



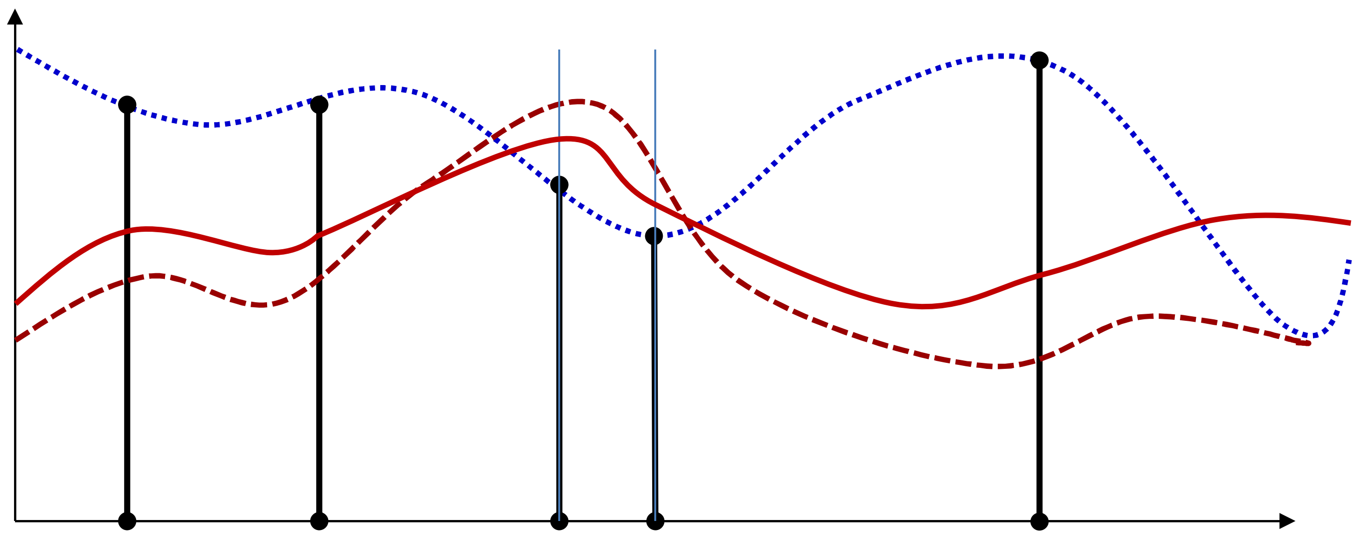
- Start with an initial function

Gradient descent



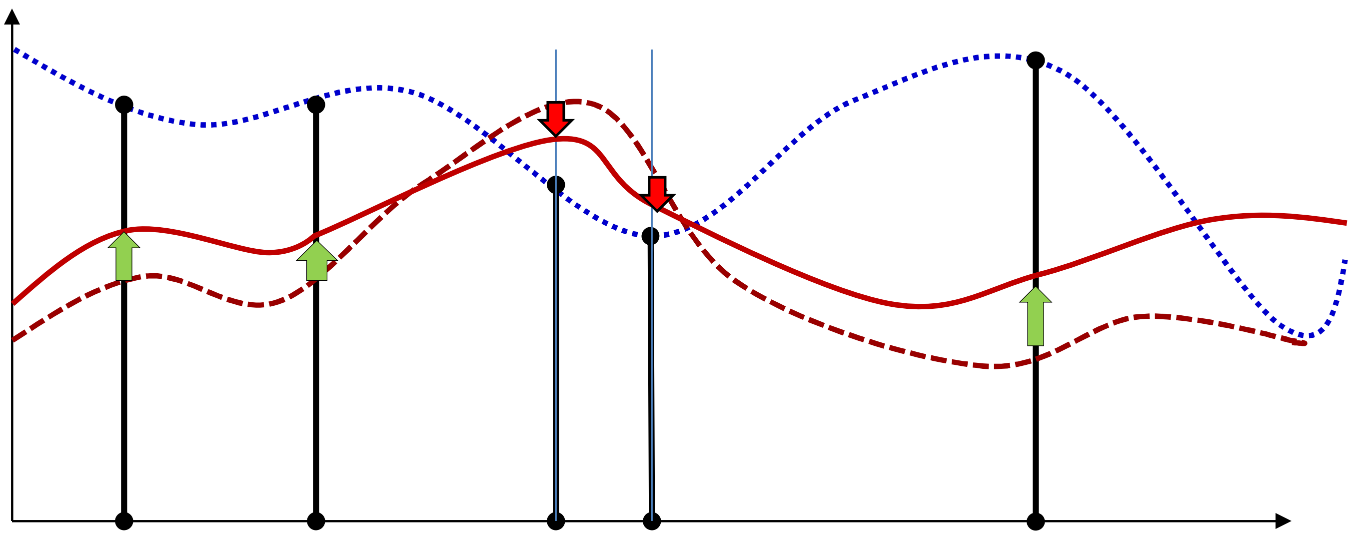
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



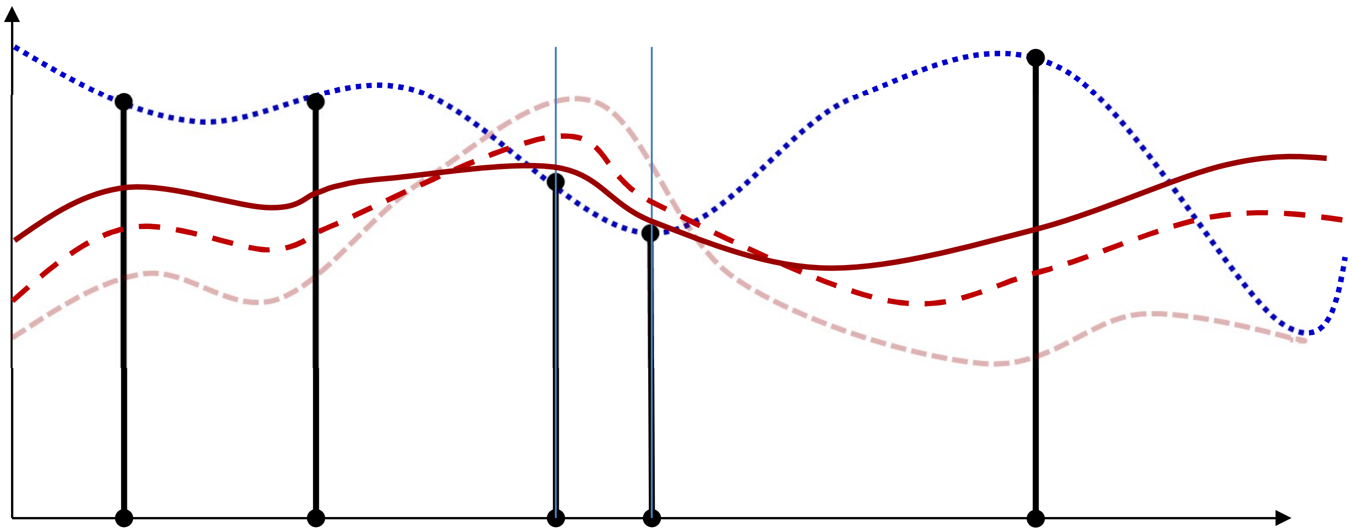
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



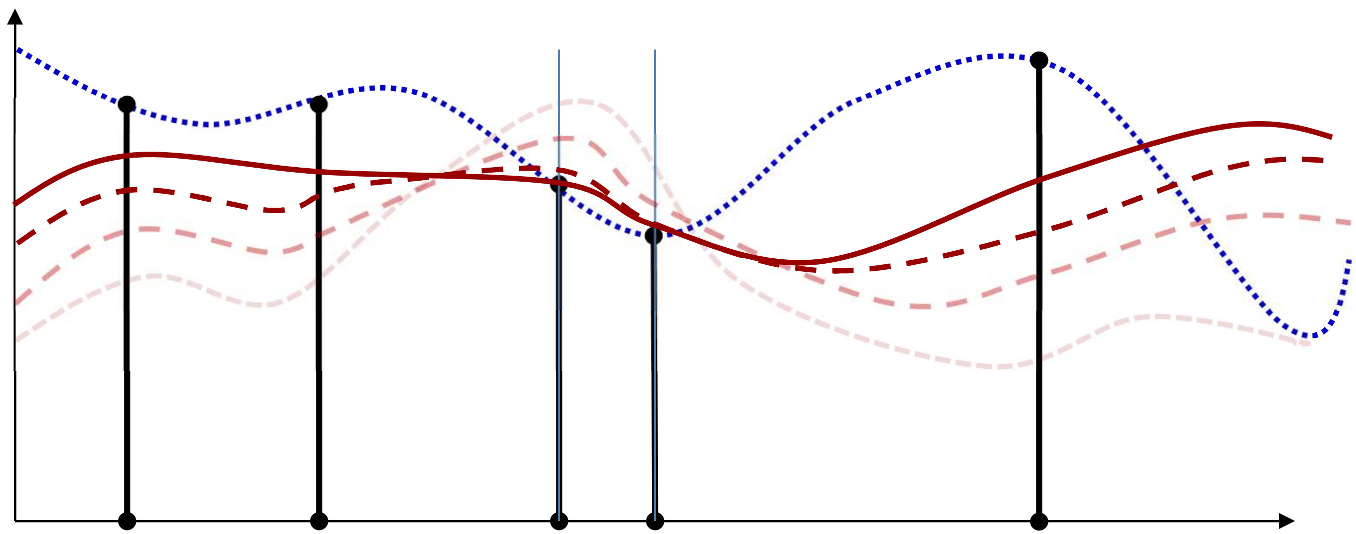
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



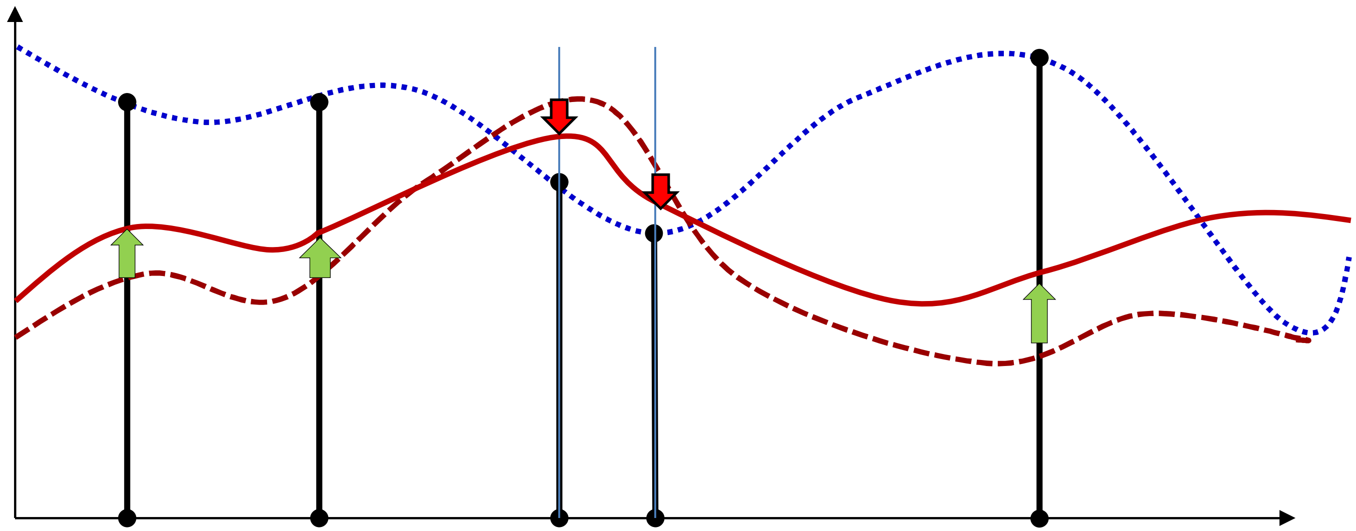
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



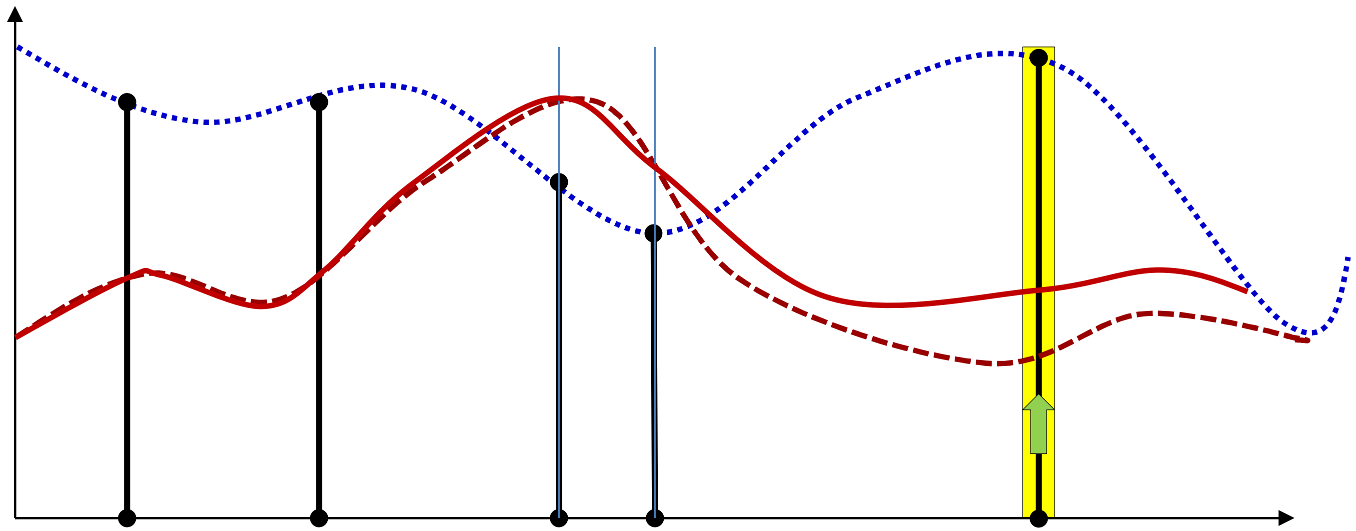
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Effect of number of samples



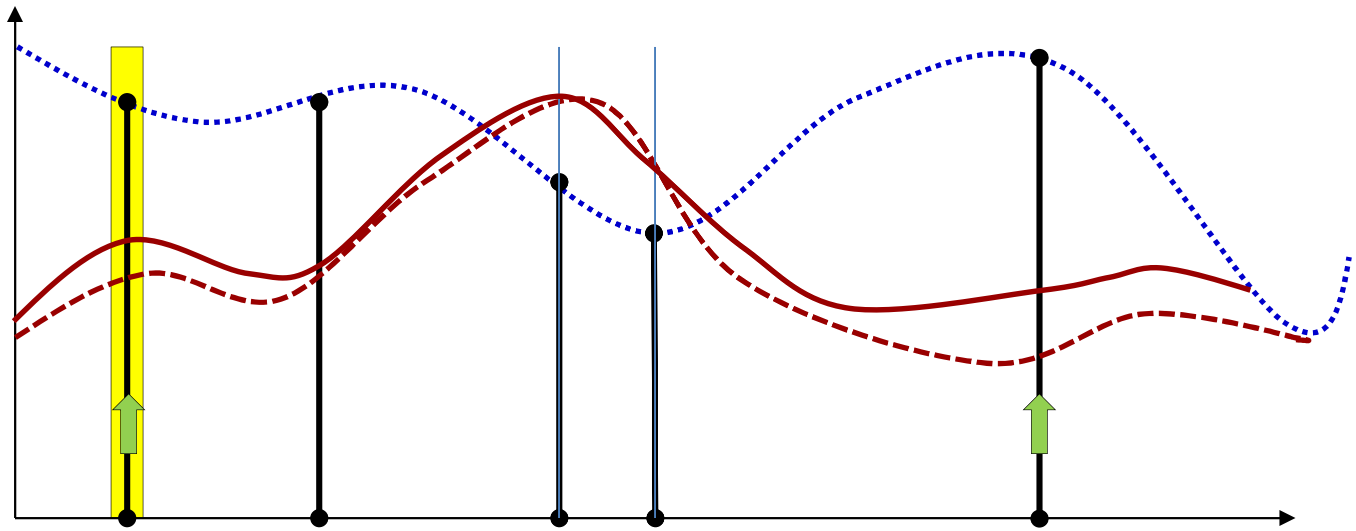
- Problem with conventional gradient descent: we try to simultaneously adjust the function at *all* training points
  - We must process *all* training points before making a single adjustment
  - **"Batch"** update

Alternative: Incremental update



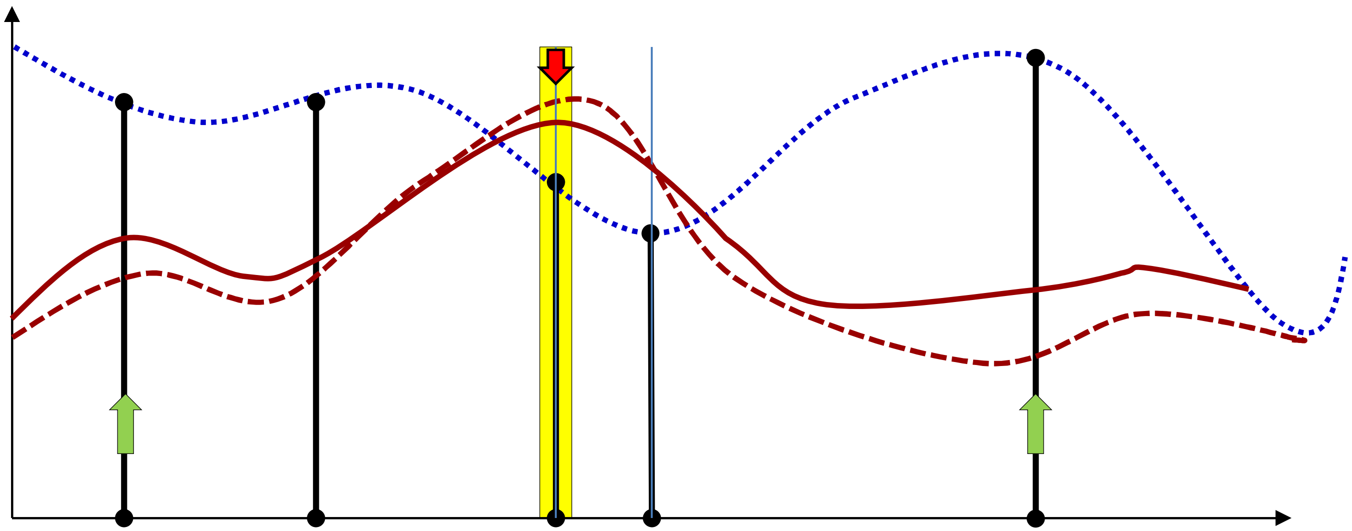
- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



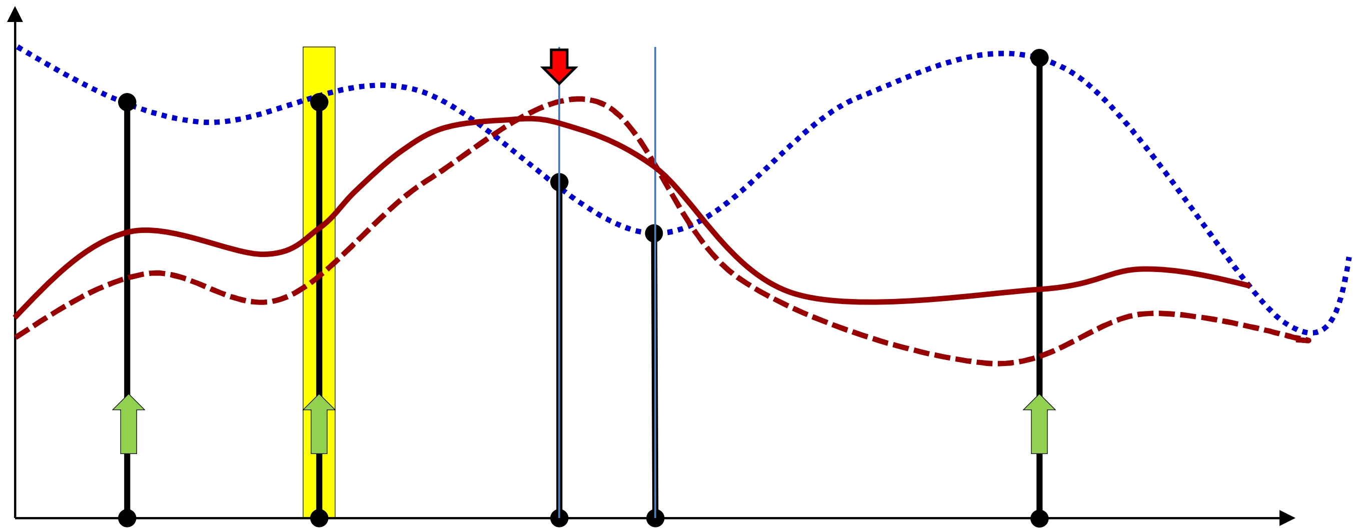
- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



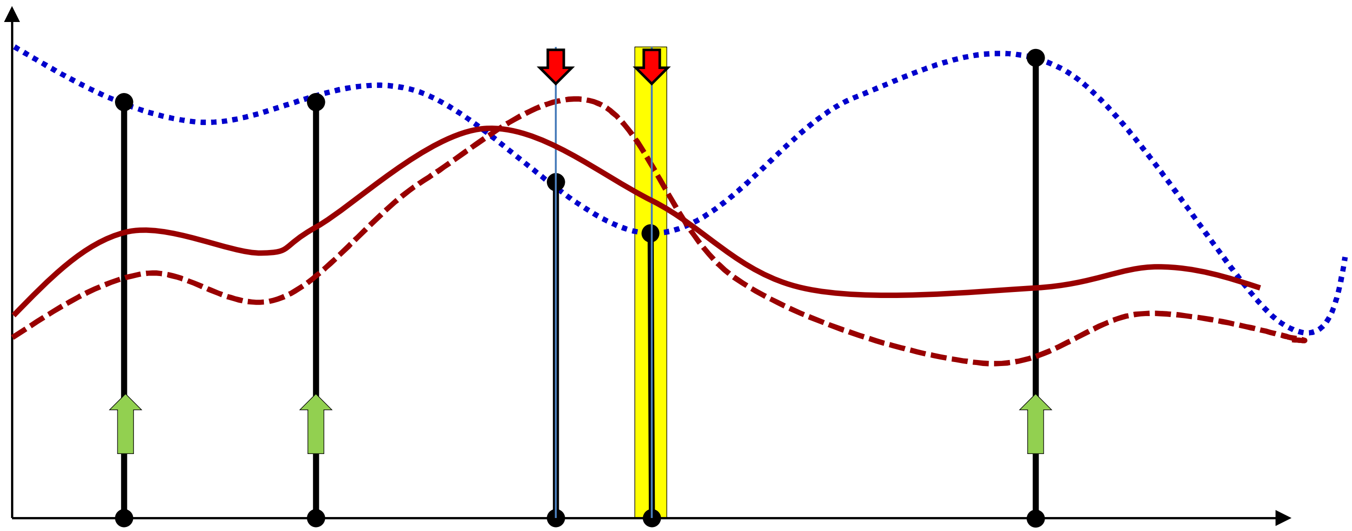
- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



- 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

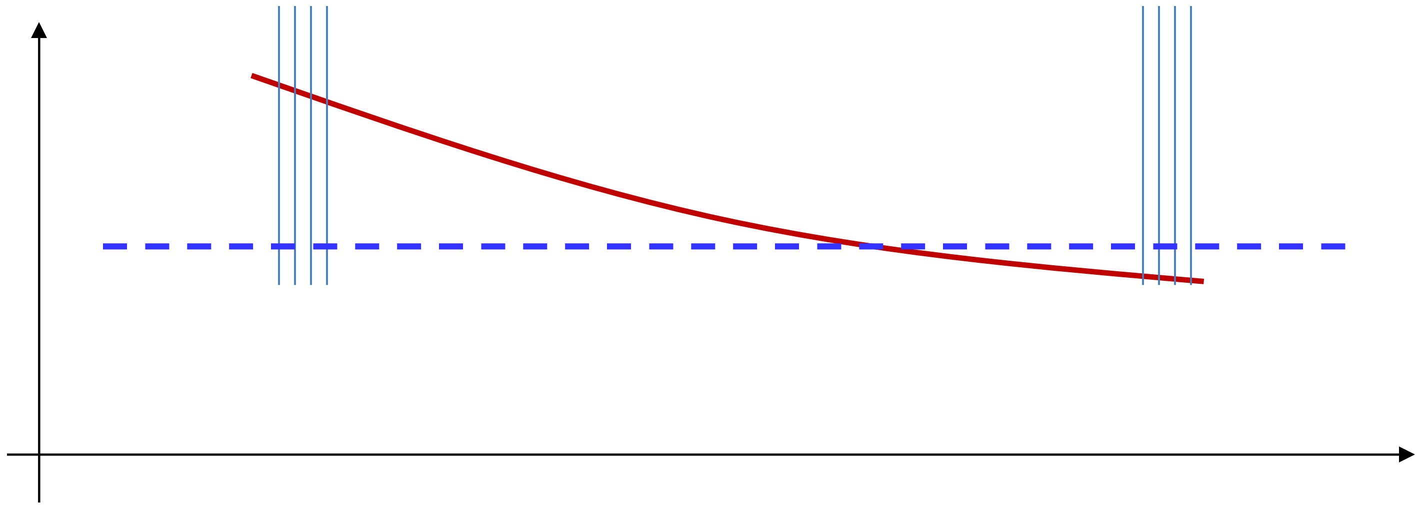
One epoch

  - For all $t = 1 : T$
    - For every layer k:
      - Compute $\nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y}_t, \boldsymbol{d}_t)$
      - Update

        $W_k = W_k - \eta \nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y}_t, \boldsymbol{d}_t)^T$ One update

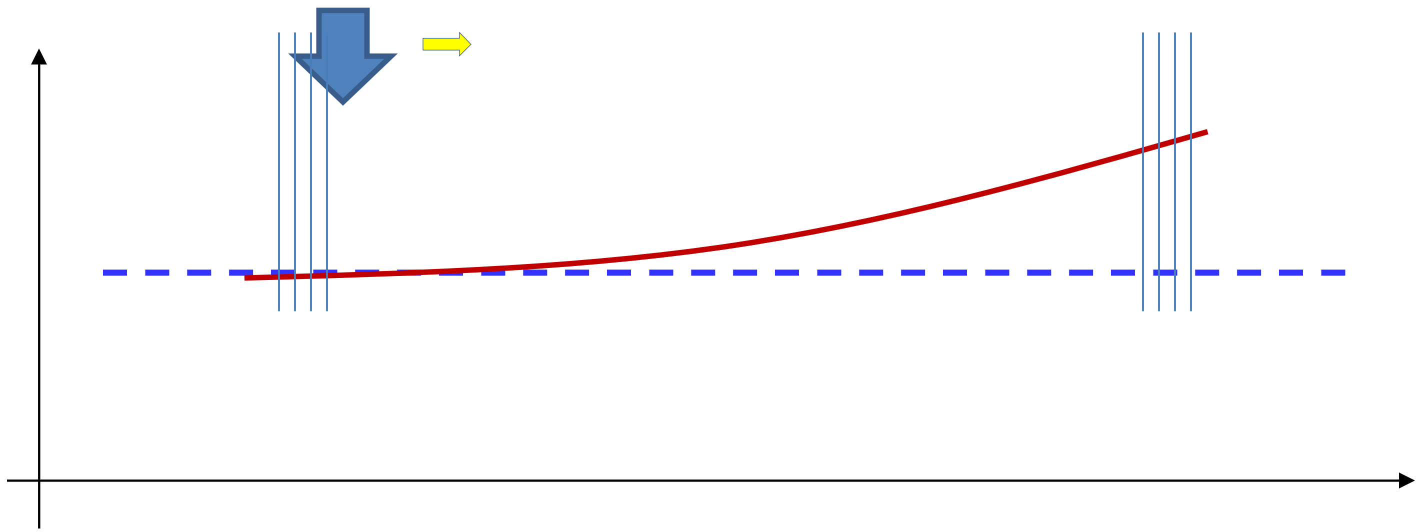
- Until $Loss$ has converged

Caveats: order of presentation



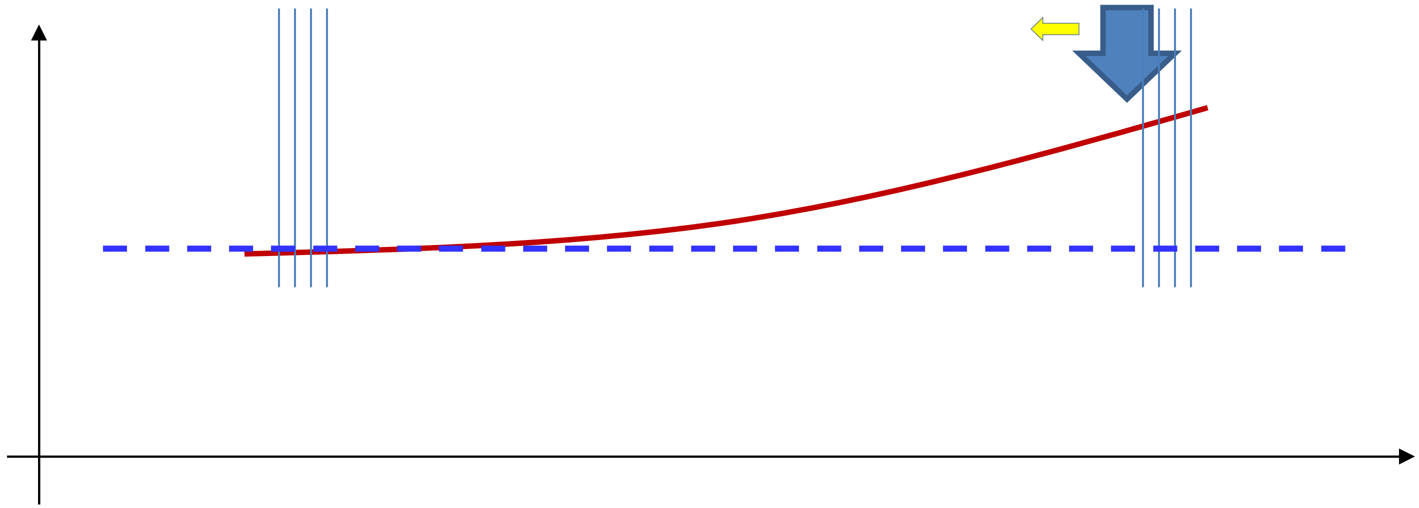
- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



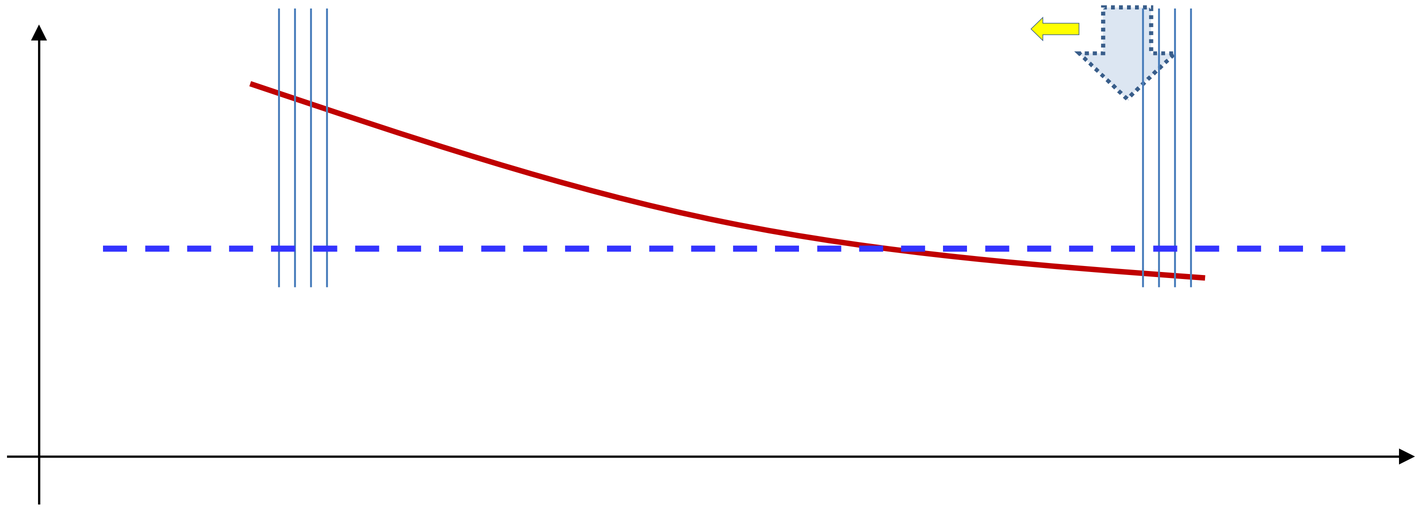
- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



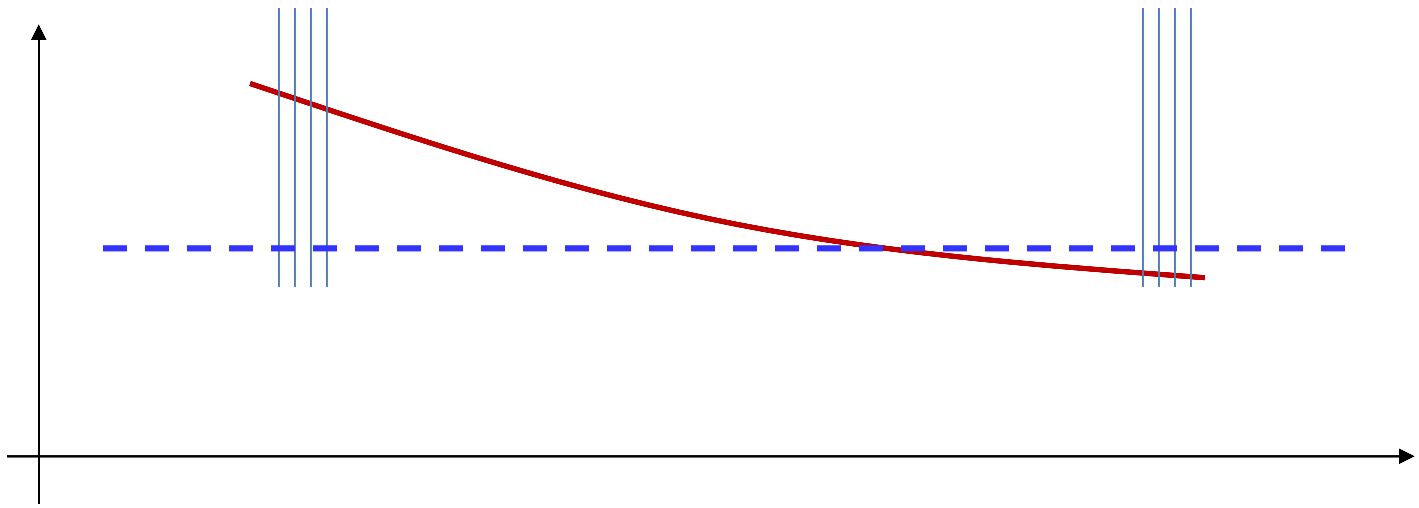
- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



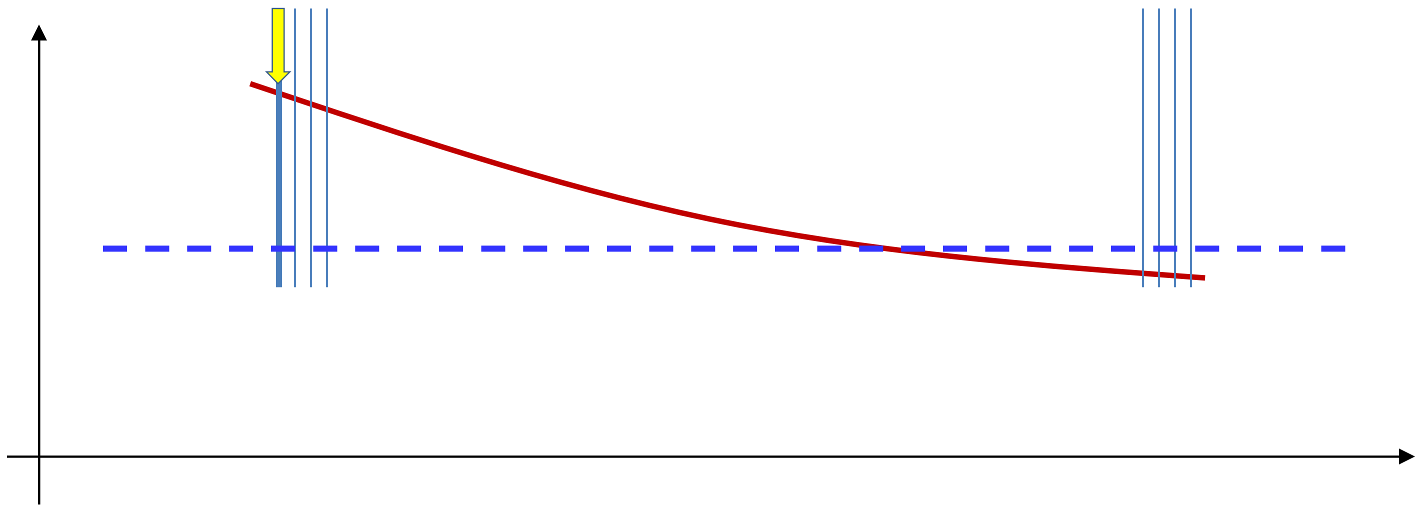
- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



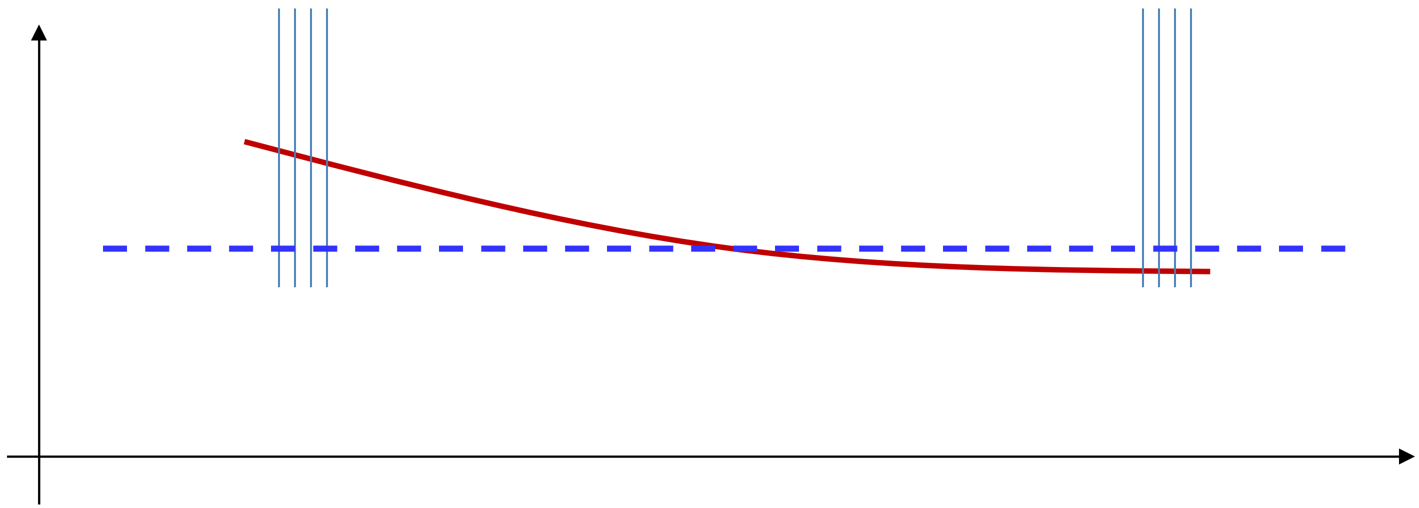
- If we loop through the samples in the same order, we may get *cyclic* behavior
- We must go through them *randomly* to get more convergent behavior

Caveats: order of presentation



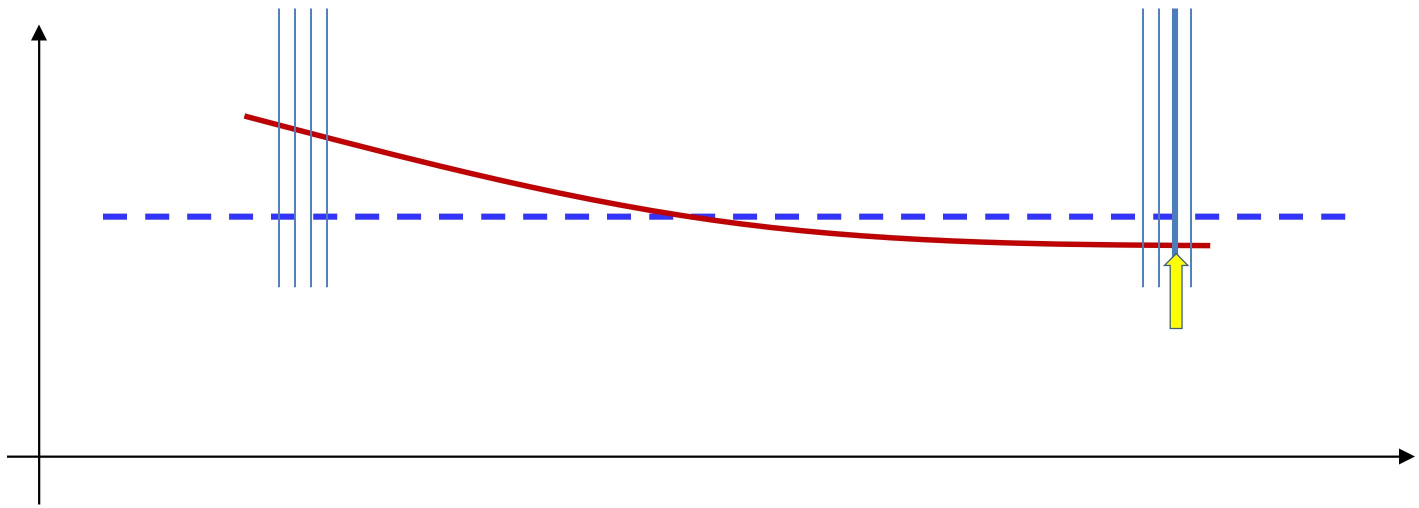
- If we loop through the samples in the same order, we may get *cyclic* behavior
- We must go through them *randomly* to get more convergent behavior

Caveats: order of presentation



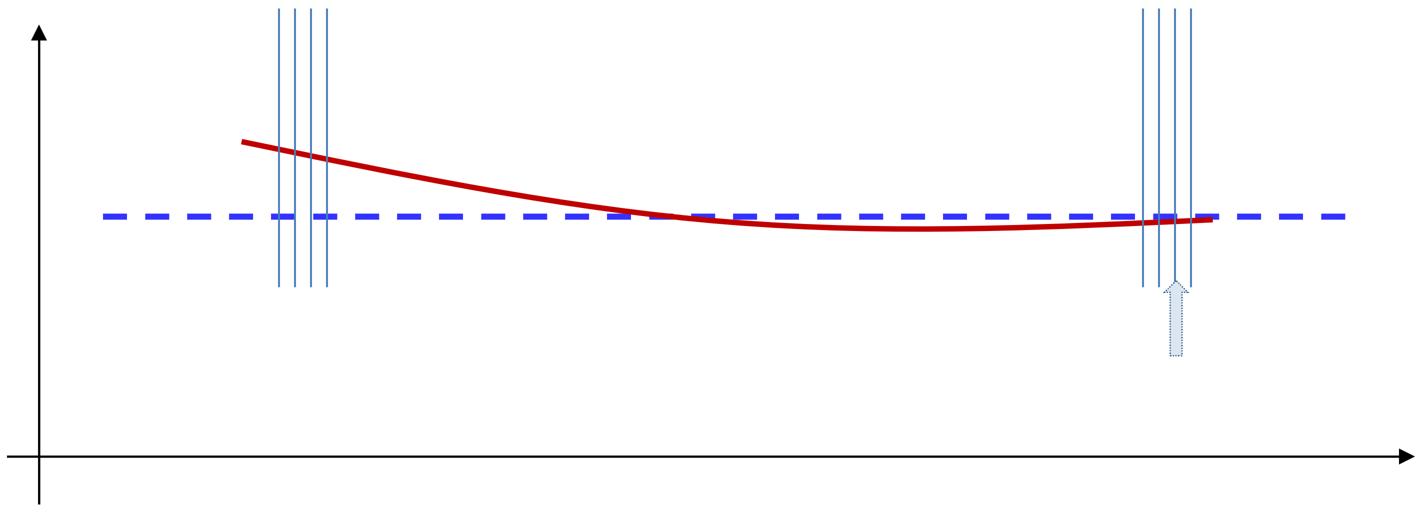
- If we loop through the samples in the same order, we may get *cyclic* behavior
- We must go through them *randomly* to get more convergent behavior

Caveats: order of presentation



- 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

Caveats: order of presentation



- 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

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:
      - 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

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

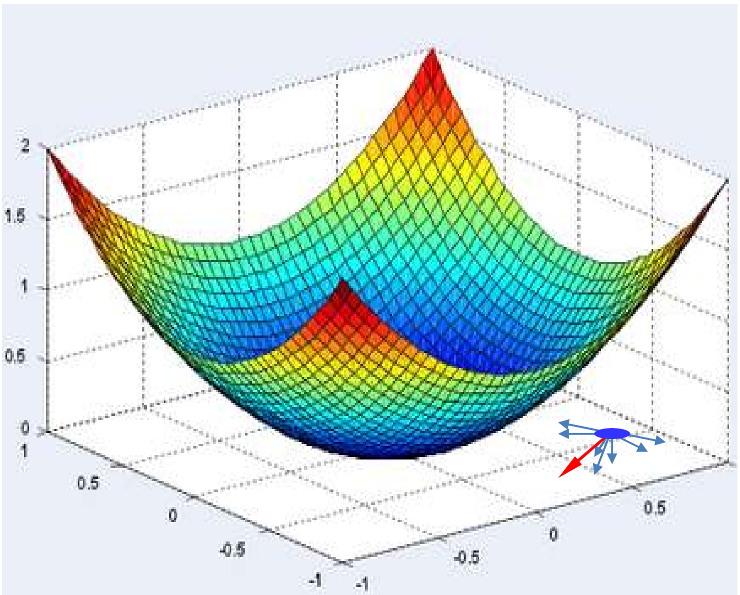
Explanations and restrictions

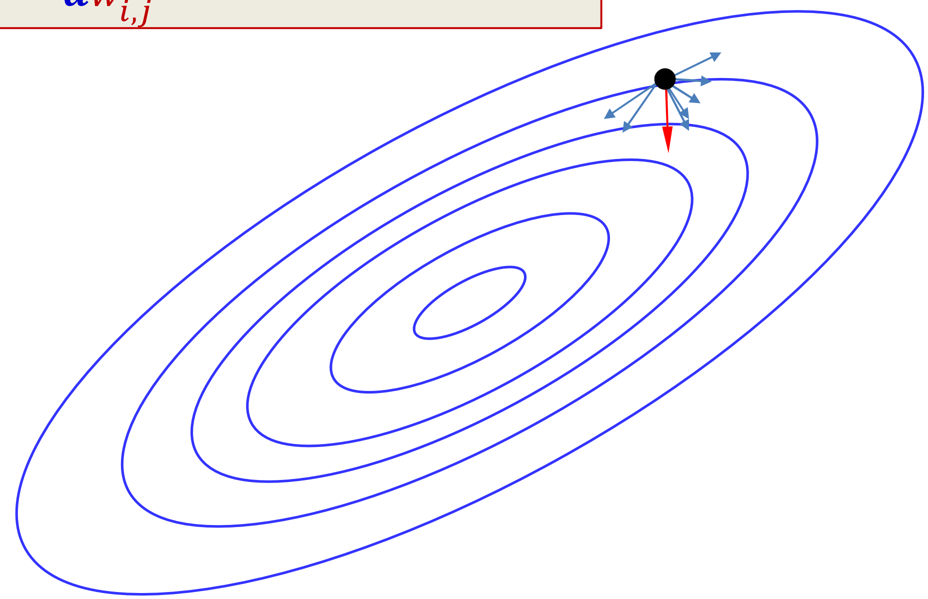
- So why does this process of incremental updates work?
- Under what conditions?

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

The expected behavior of the gradient

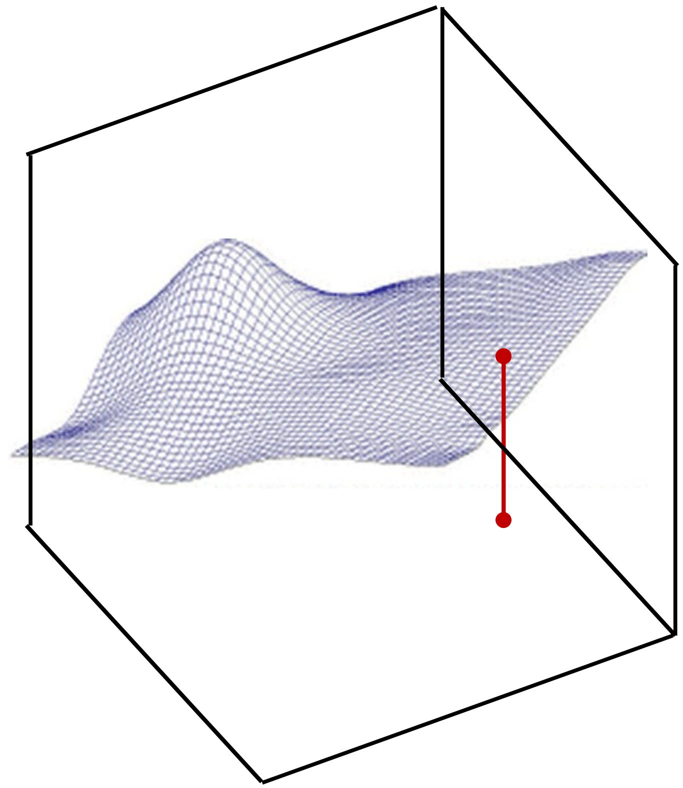
$$\frac{dE(\boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}, \dots, \boldsymbol{W}^{(K)})}{dw_{i,j}^{(k)}} = \frac{1}{T}\sum_i \frac{dDiv(\boldsymbol{Y}(\boldsymbol{X}_i), \boldsymbol{d}_i; \boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}, \dots, \boldsymbol{W}^{(K)})}{dw_{i,j}^{(k)}}$$





- 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

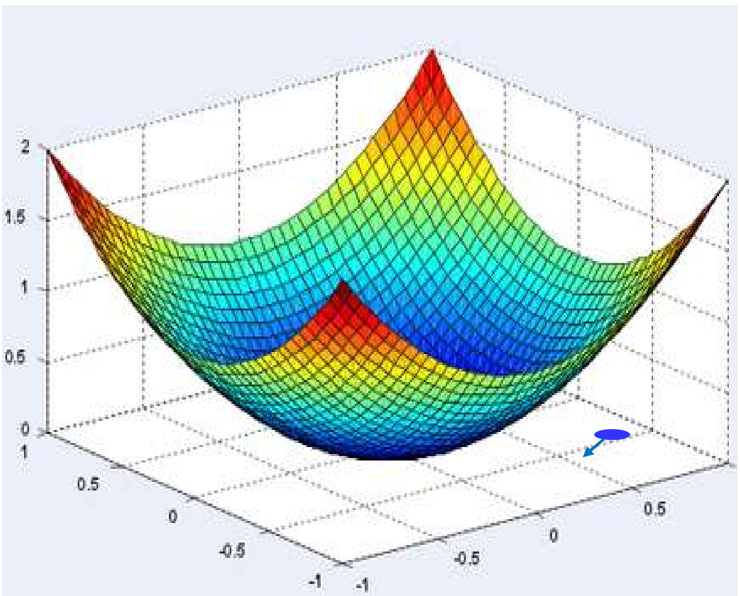


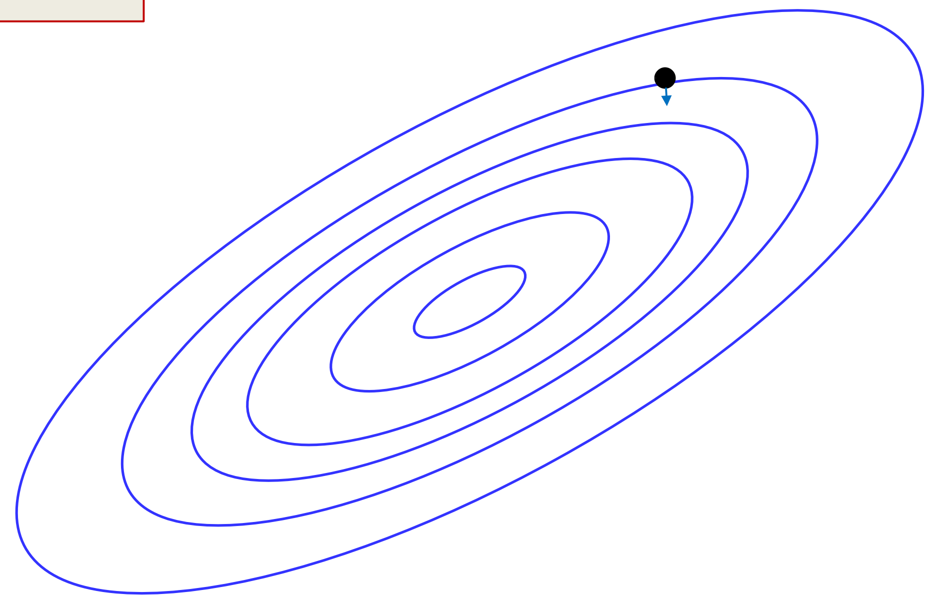
$$X_1 = X_2 = \cdots = X_T$$

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

The expected behavior of the gradient

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

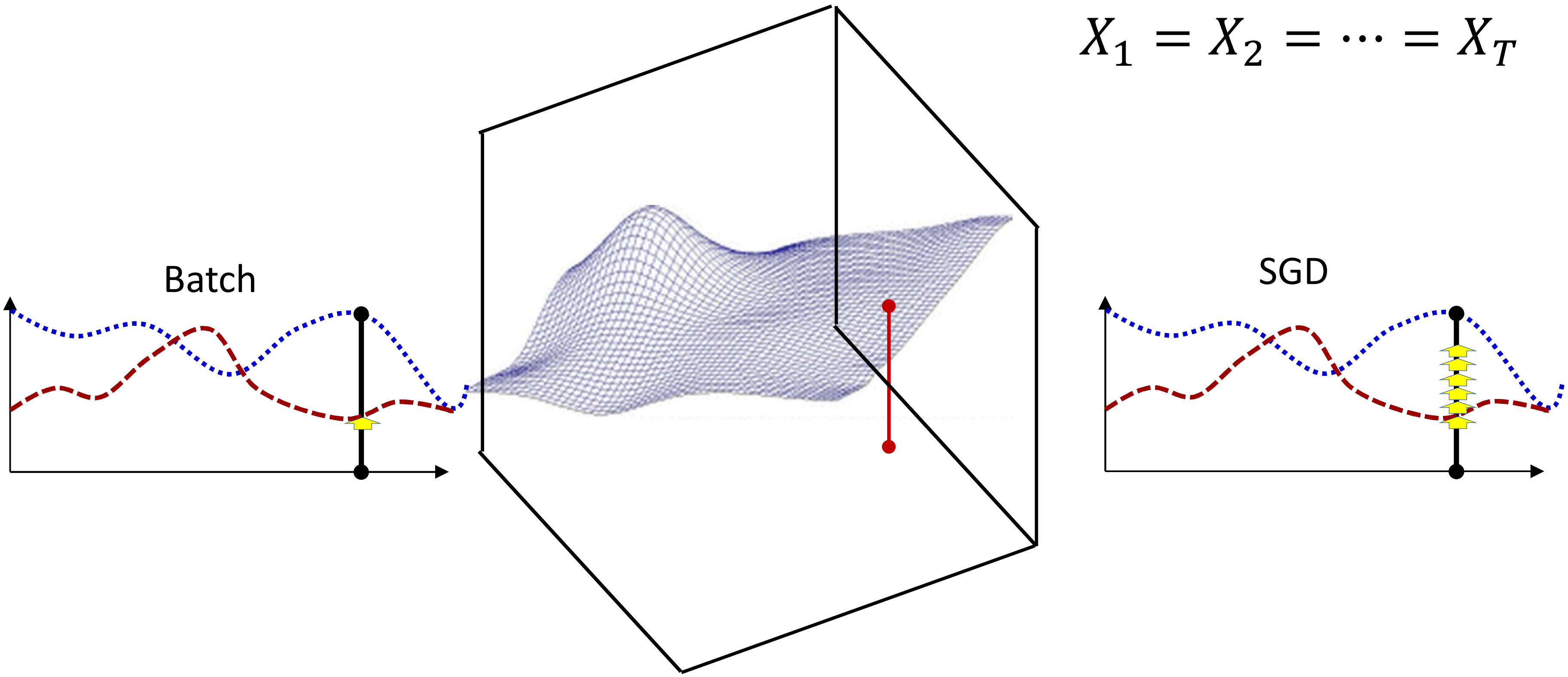




- The individual training instance contribute identical directions to the overall gradient
  - The final gradient points is simply the gradient for an individual instance

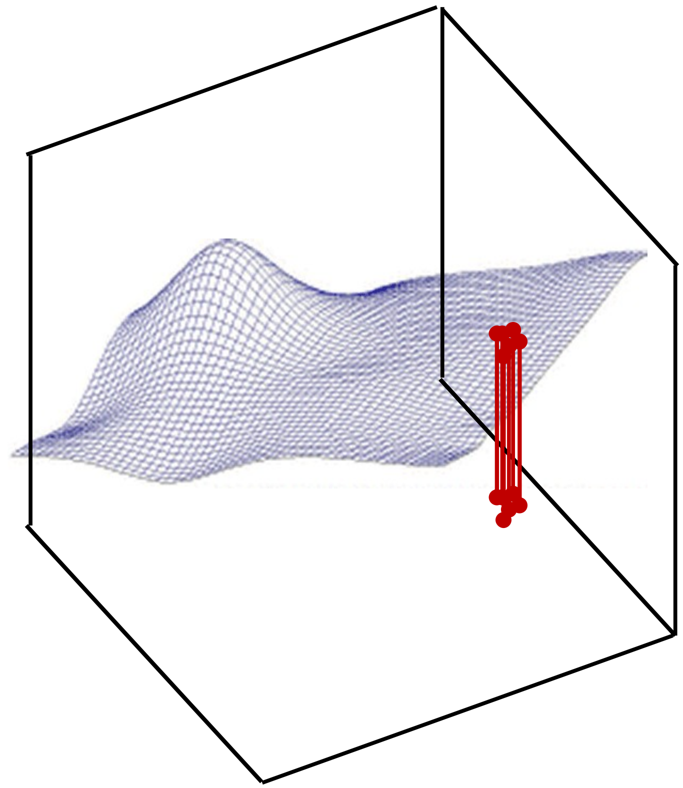
Batch vs SGD

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



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

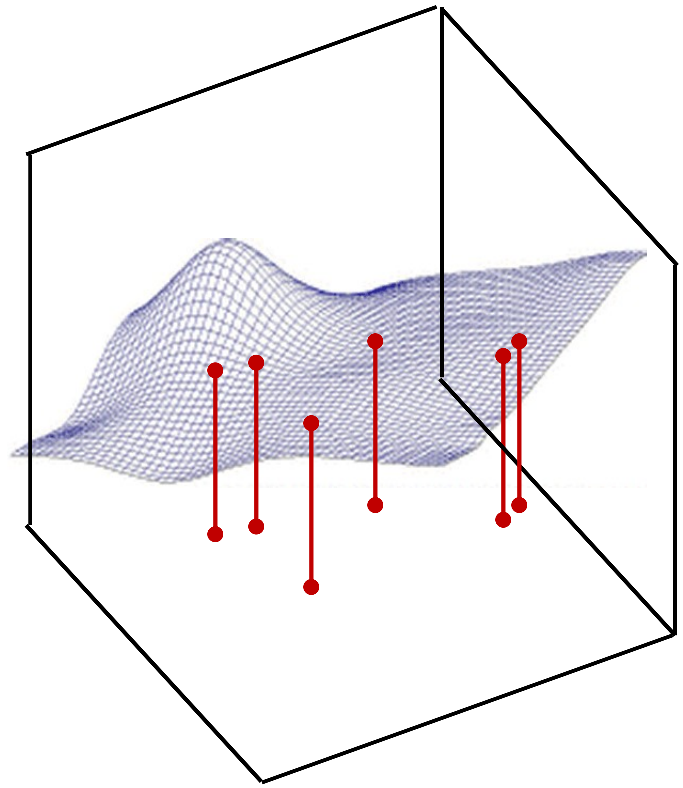
Clumpy data..



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

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

Clumpy data..



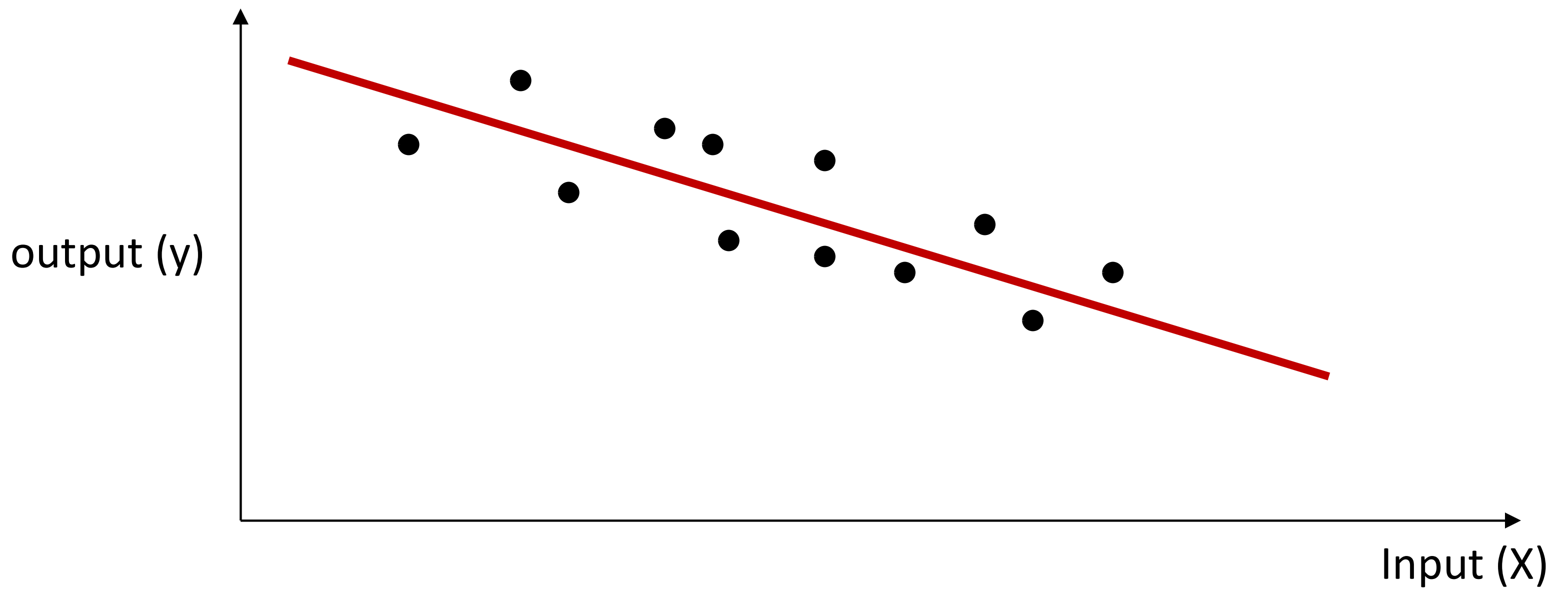
- As data get increasingly diverse, the benefits of incremental updates decrease, but do not entirely vanish

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

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

Randomize input order

Learning rate reduces with j

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

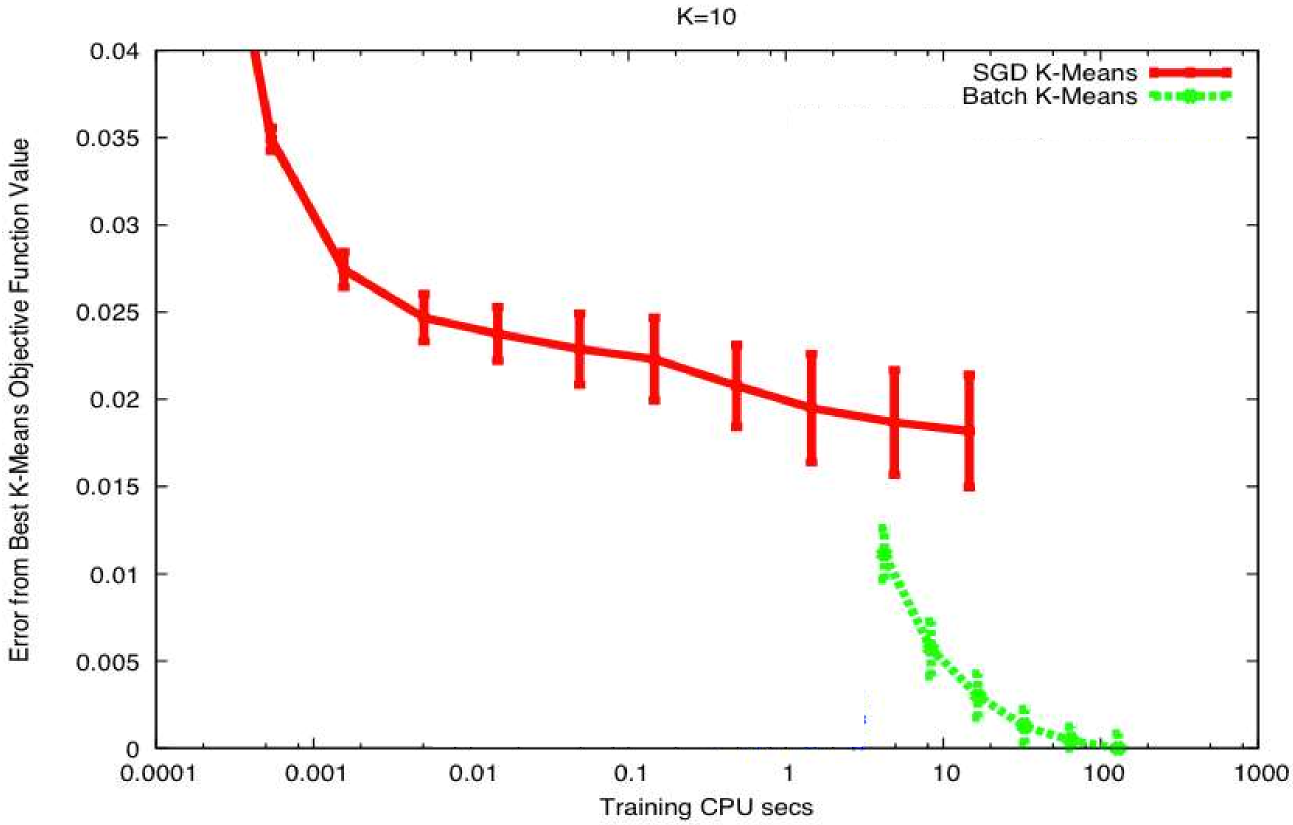
Polynomial Decay Averaging:

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

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

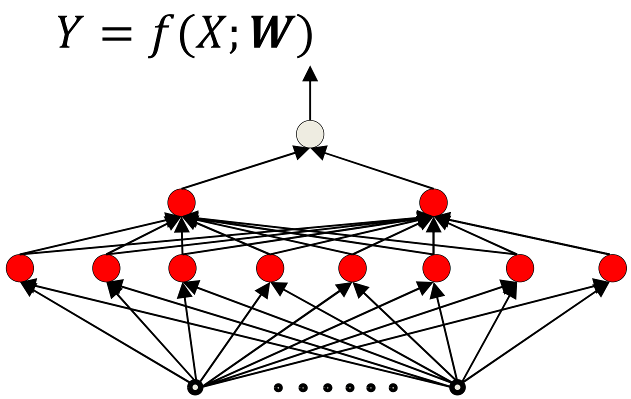
Achieves $\mathcal{O}\left(\frac{1}{T}\right)$ (strongly convex) and $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ (convex) convergence

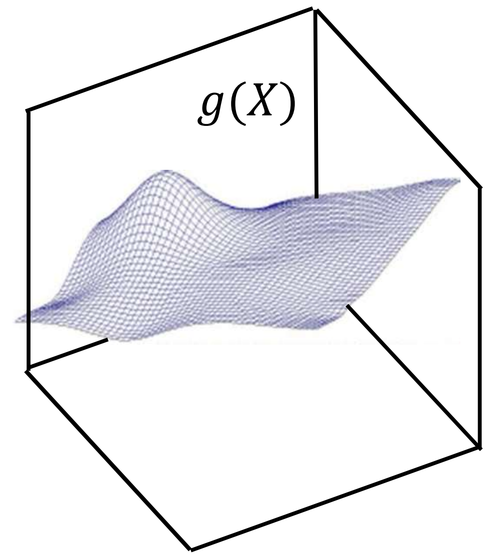
SGD example



- A simpler problem: K-means
- Note: SGD converges slower
- Also note the rather large variation between runs
  - Lets try to understand these results..

Recall: Modelling a function



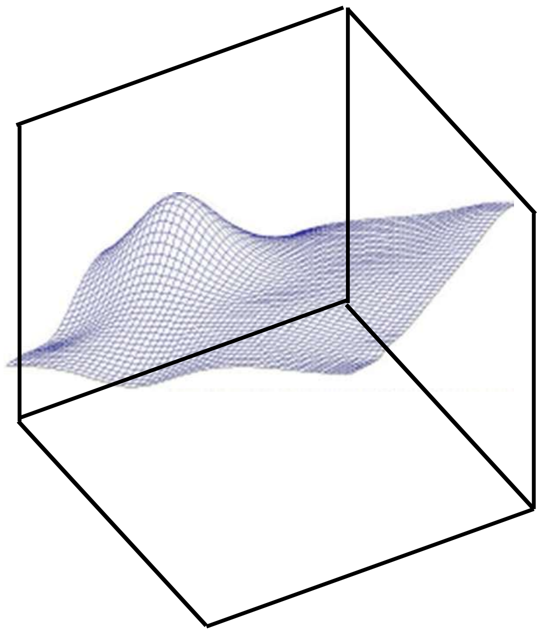


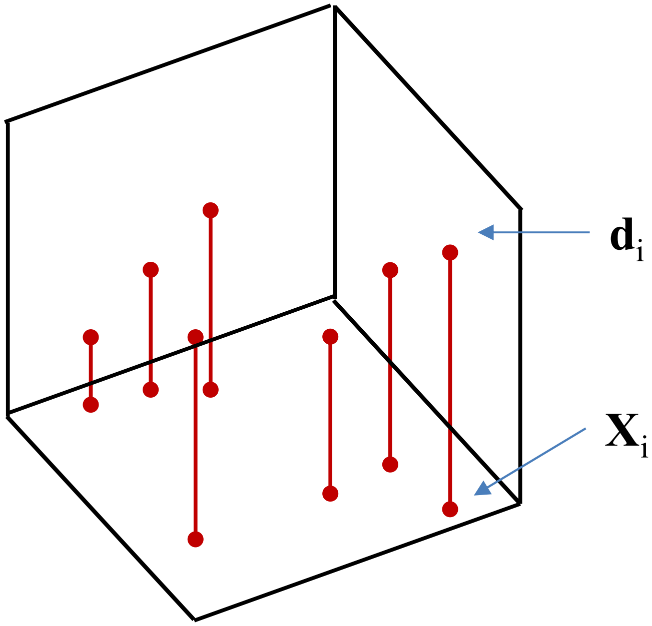
- To learn a network $f(X; \boldsymbol{W})$ to model a function $g(X)$ we minimize the *expected divergence*

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

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

Recall: The *Empirical* risk





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

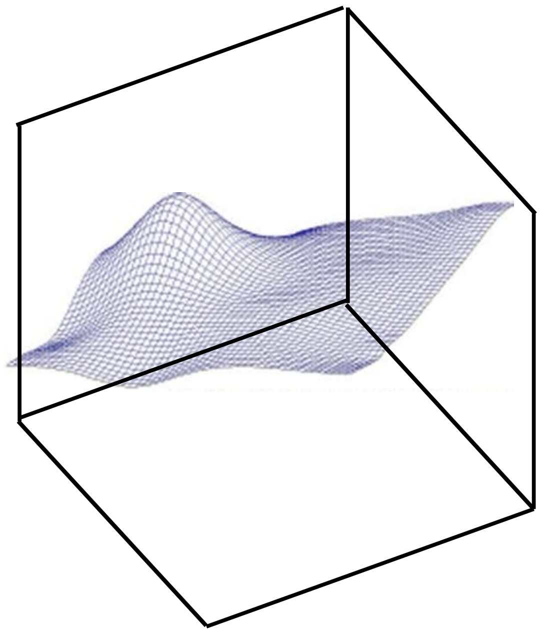
$$Loss(W) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i;W),d_i)$$

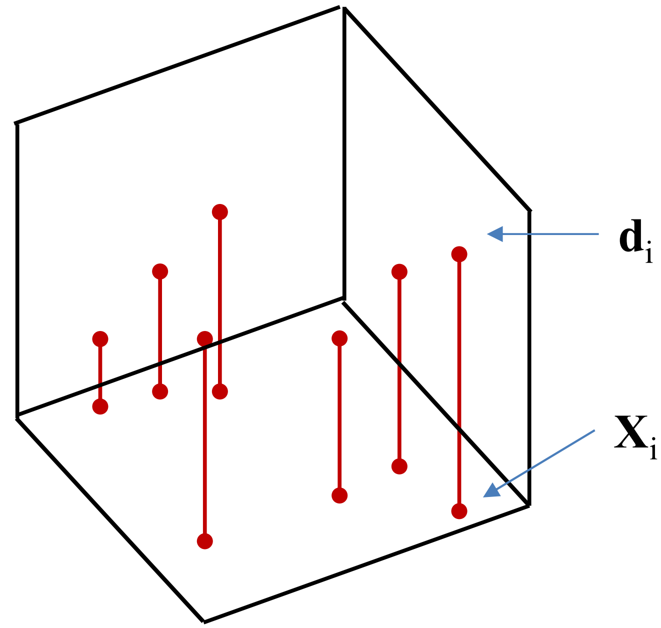
$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}}\, Loss(W)$$

- 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)*

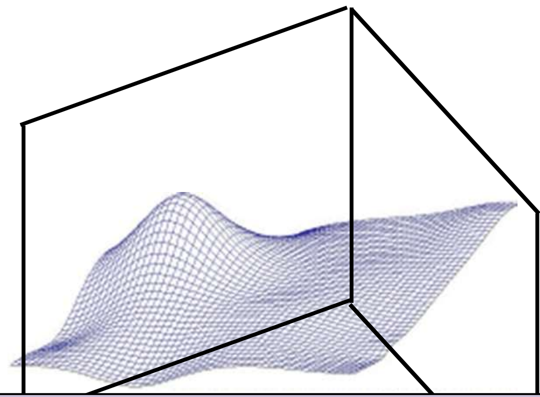
$$Loss(W) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i; W), d_i)$$

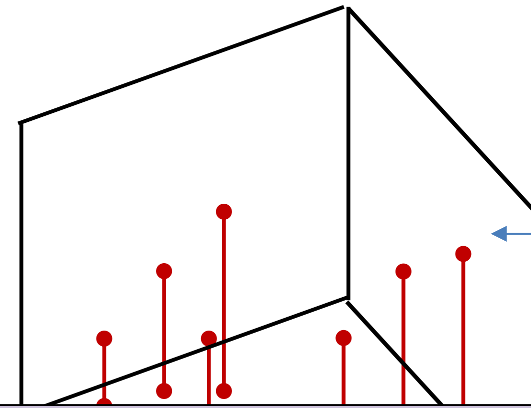
The empirical risk is an *unbiased* estimate of the expected divergence

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

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

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

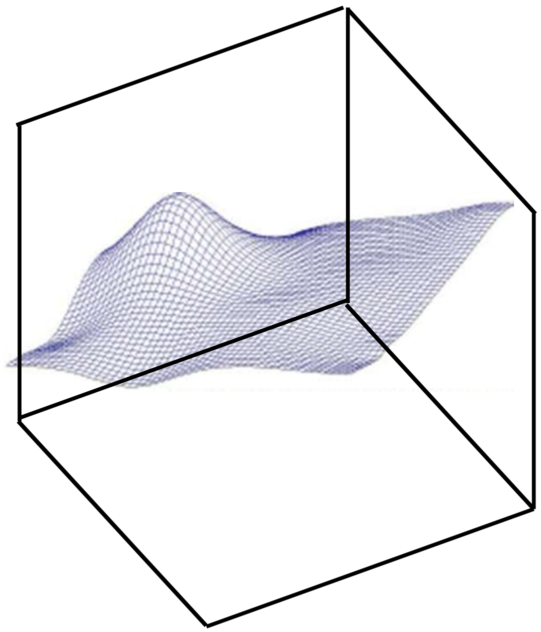
$$Loss(W) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i; W), d_i)$$

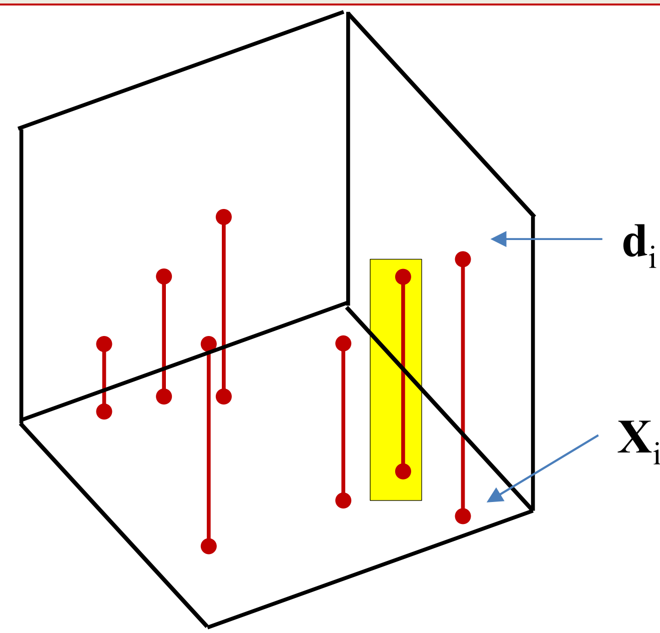
The empirical risk is an *unbiased* estimate of the expected divergence

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

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

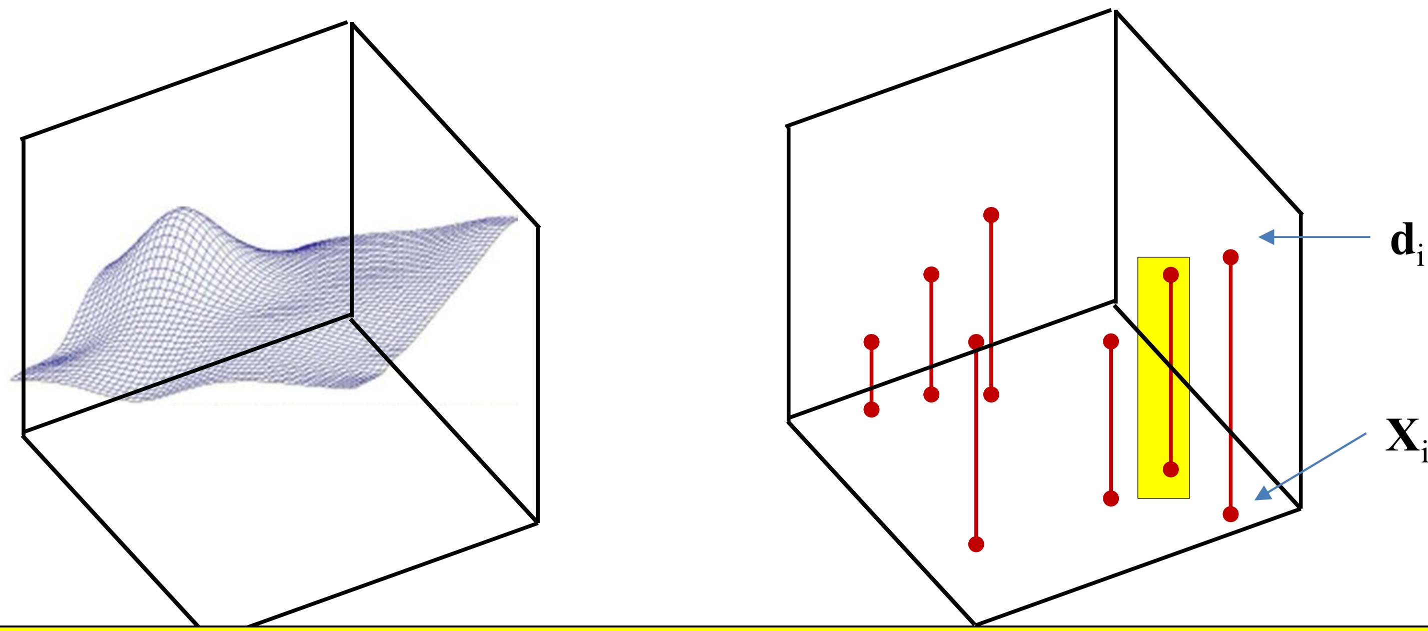
SGD





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

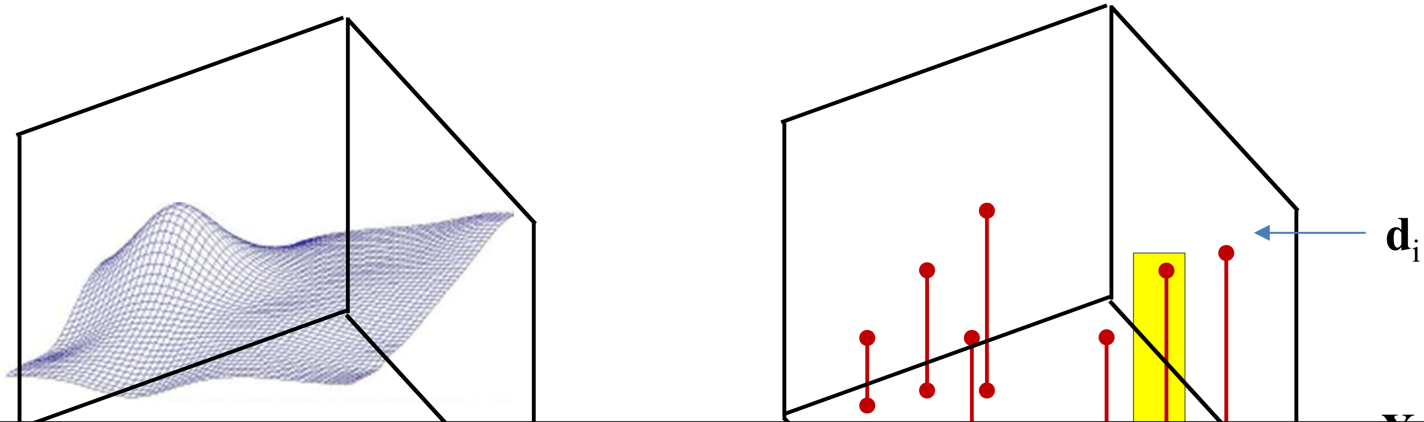
SGD



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

- 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

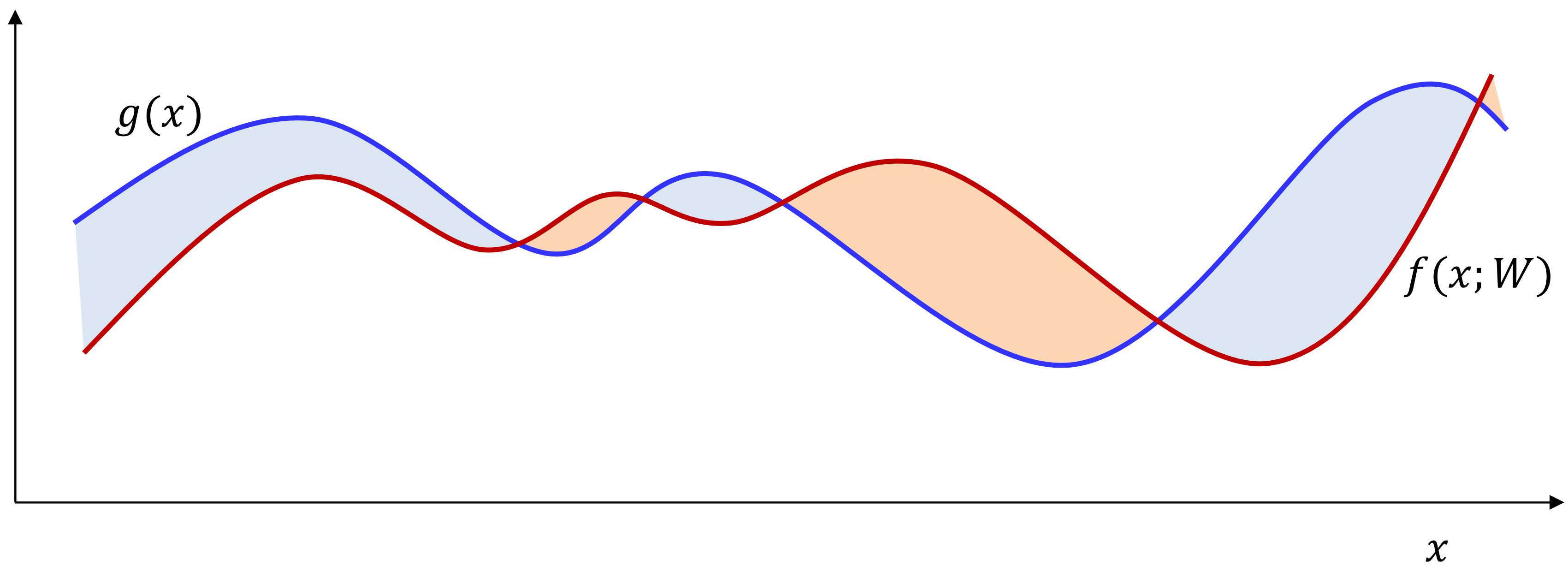


The variance of the sample divergence is the variance of the divergence itself: var(div). This is N times the variance of the empirical average minimized by batch update

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

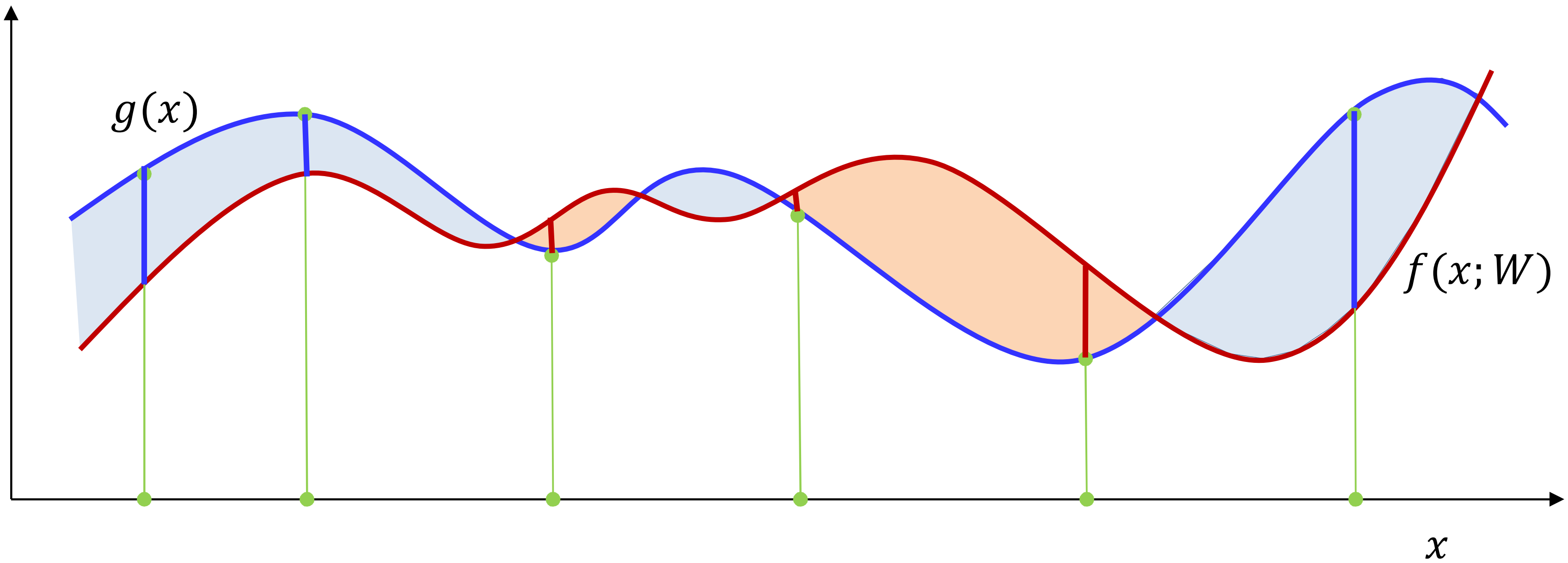
- At each iteration, **SGD** focuses on the divergence of a ***single*** sample $div(f(X_i; W), d_i)$
- The *expected value* of the *sample error* is ***still*** the *expected divergence* $E\left[div\left(f(X; W), g(X)\right)\right]$

Explaining the variance



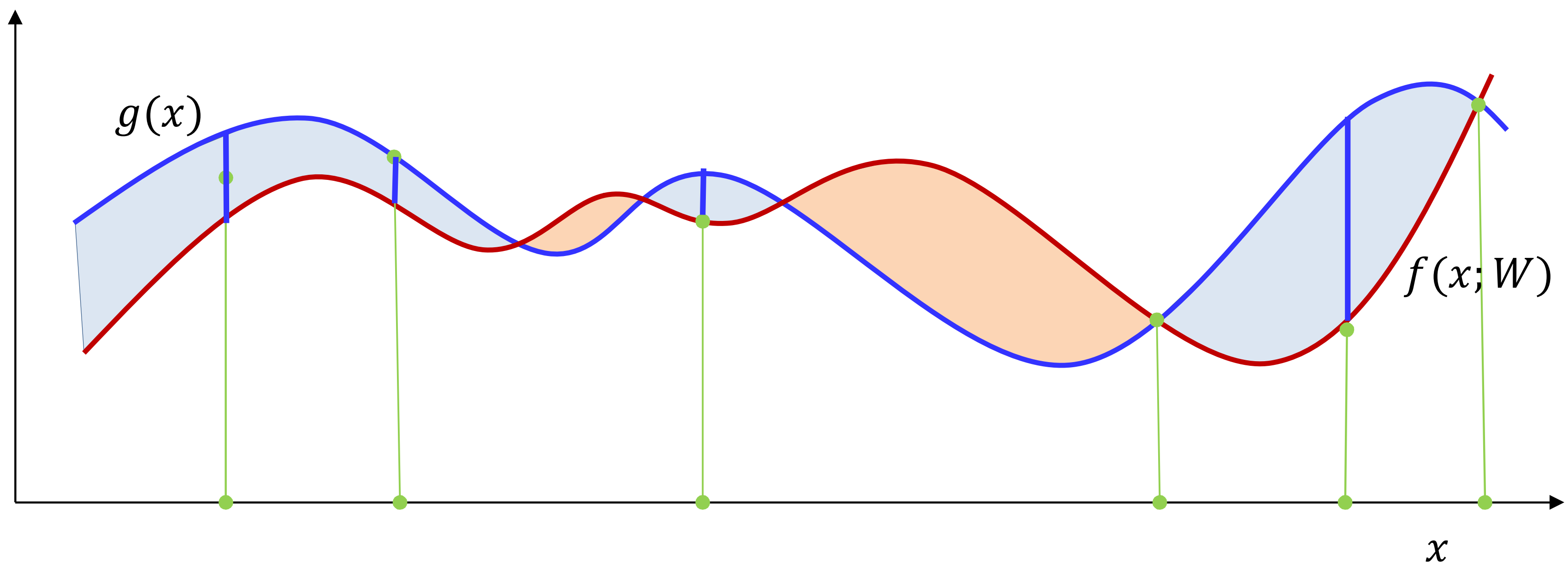
- The blue curve is the function being approximated
- The red curve is the approximation by the model at a given W
- The heights of the shaded regions represent the point-by-point error
  - The divergence is a function of the error
  - We want to find the W that minimizes the average divergence

Explaining the variance



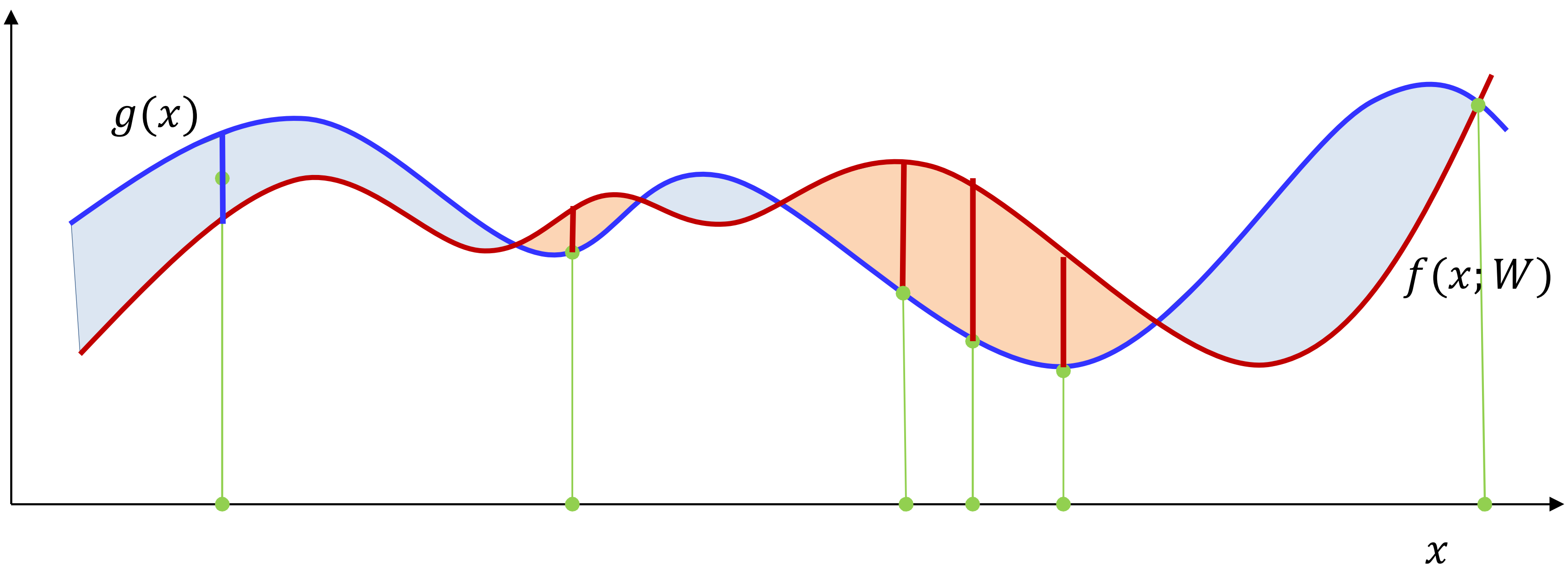
- Sample estimate approximates the shaded area with the average length of the lines

Explaining the variance



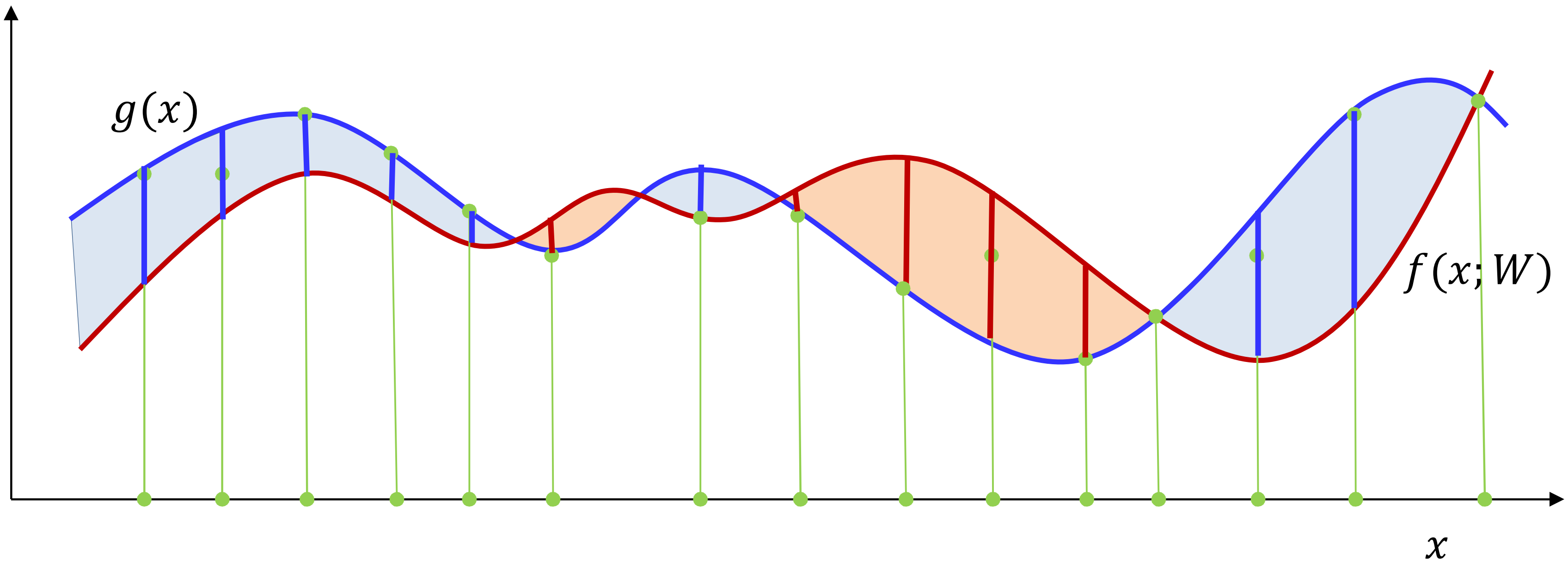
- Sample estimate approximates the shaded area with the average length of the lines
- This average length will change with position of the samples

Explaining the variance



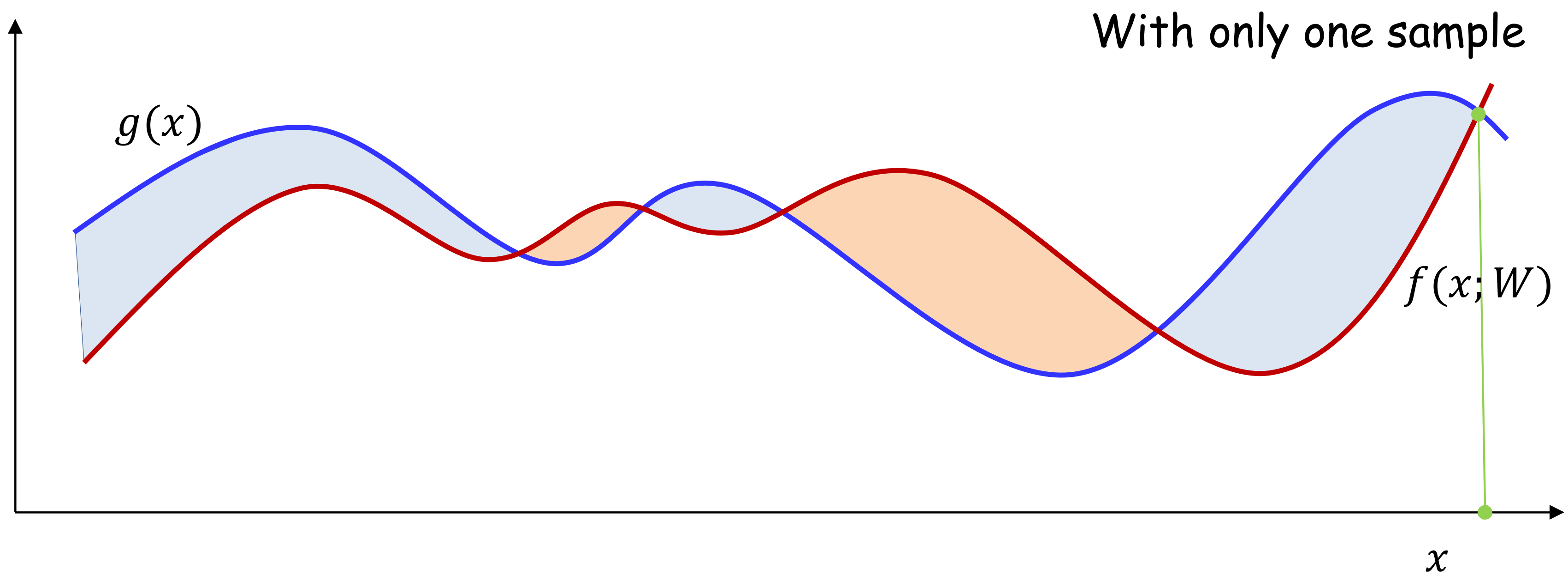
- Sample estimate approximates the shaded area with the average length of the lines
- This average length will change with position of the samples

Explaining the variance



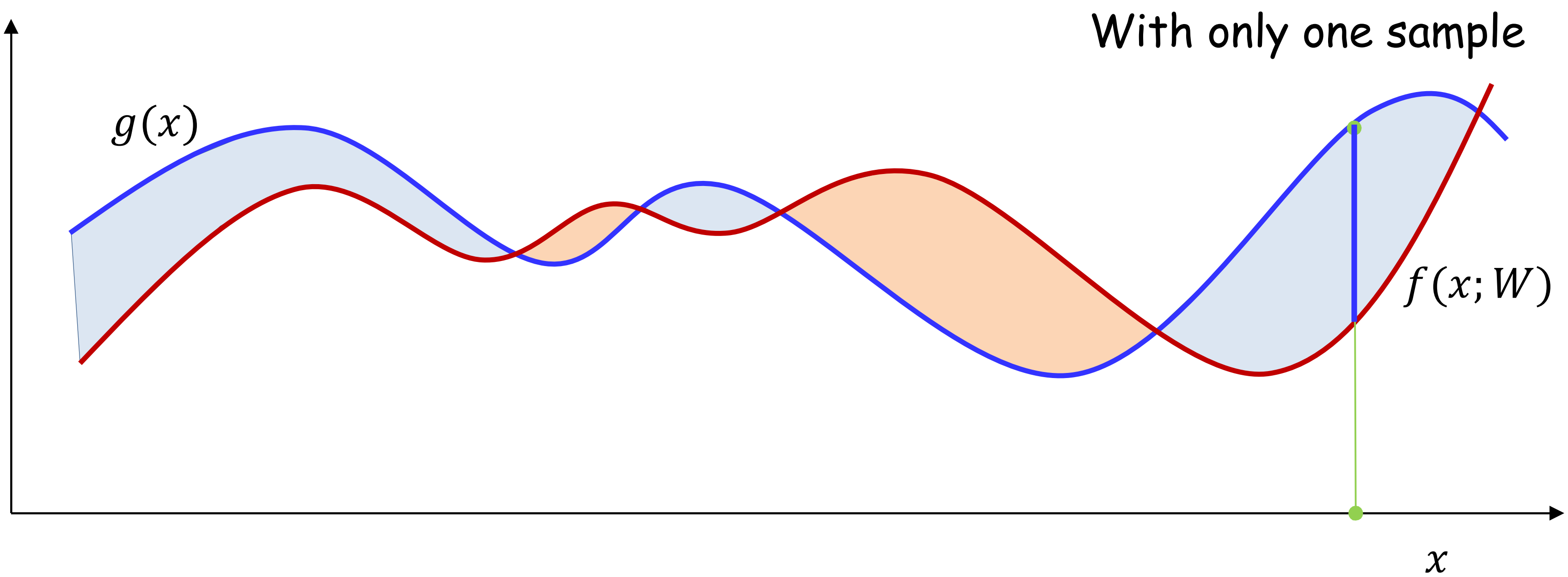
- Having more samples makes the estimate more robust to changes in the position of samples
  - The variance of the estimate is smaller

Explaining the variance



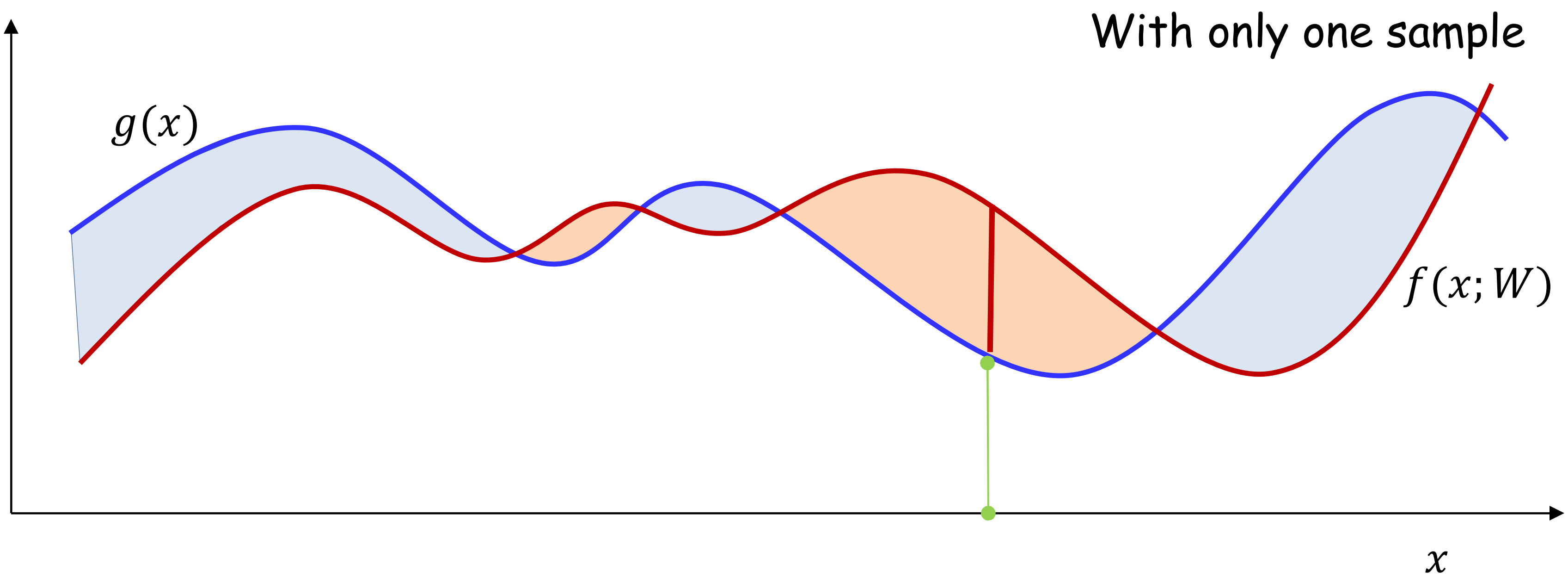
- Having very few samples makes the estimate swing wildly with the sample position
  - Since our estimator learns the W to minimize this estimate, the learned W too can swing wildly

Explaining the variance



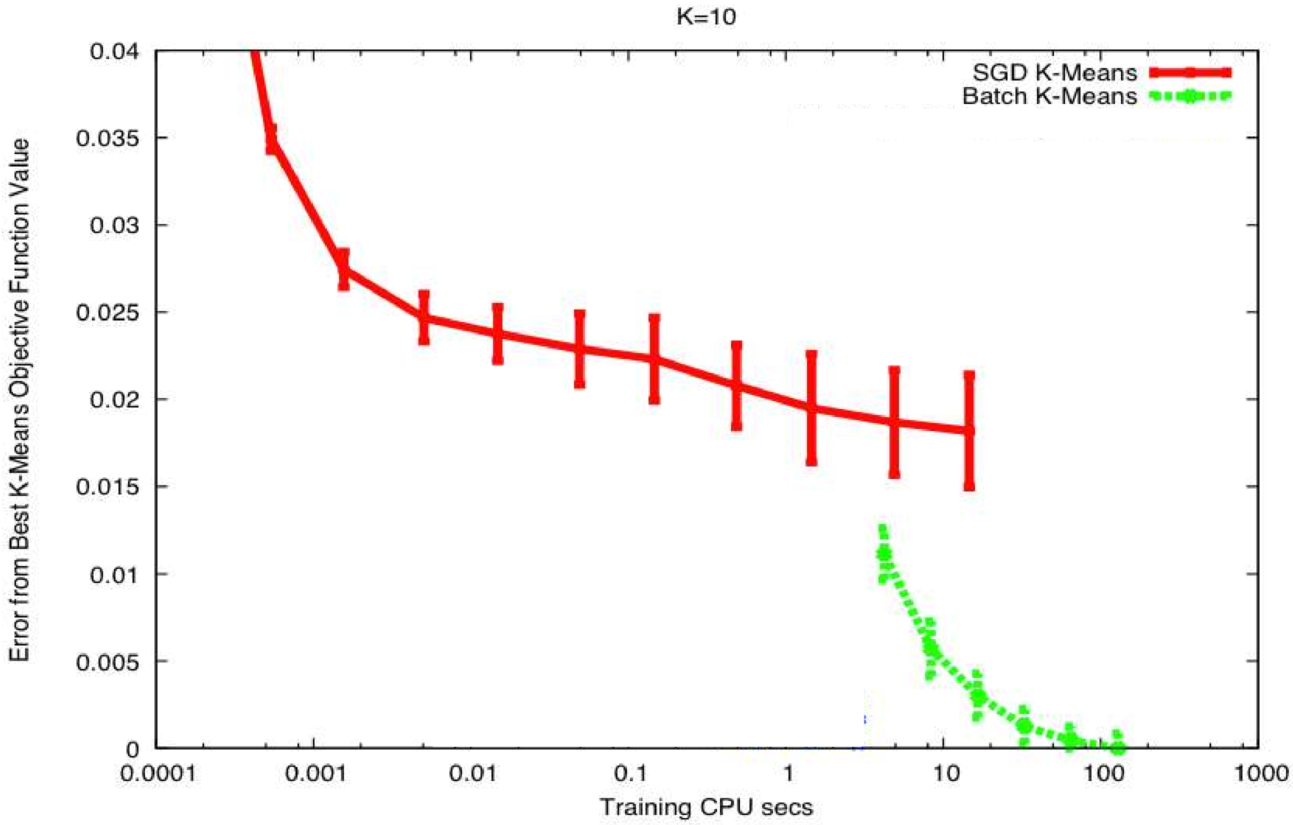
- Having very few samples makes the estimate swing wildly with the sample position
  - Since our estimator learns the W to minimize this estimate, the learned W too can swing wildly

Explaining the variance



- 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

SGD example



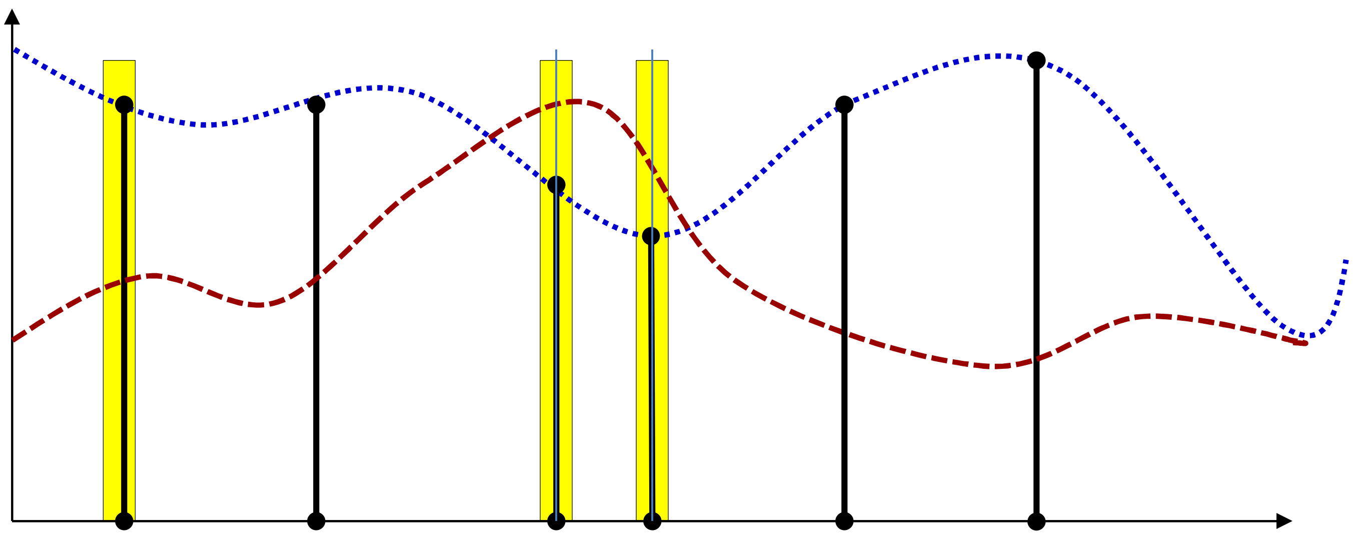
- A simpler problem: K-means
- Note: SGD converges slower
- Also has large variation between runs

SGD vs batch

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

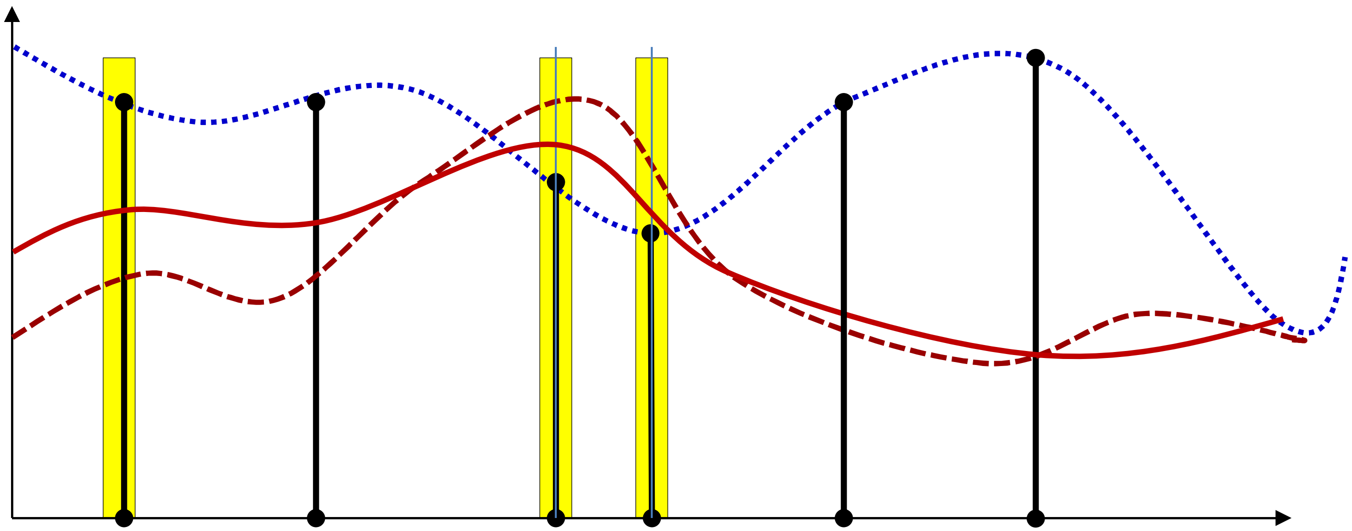
- But also provides significantly quicker updates than batch
- Is there a good medium?

Alternative: Mini-batch update



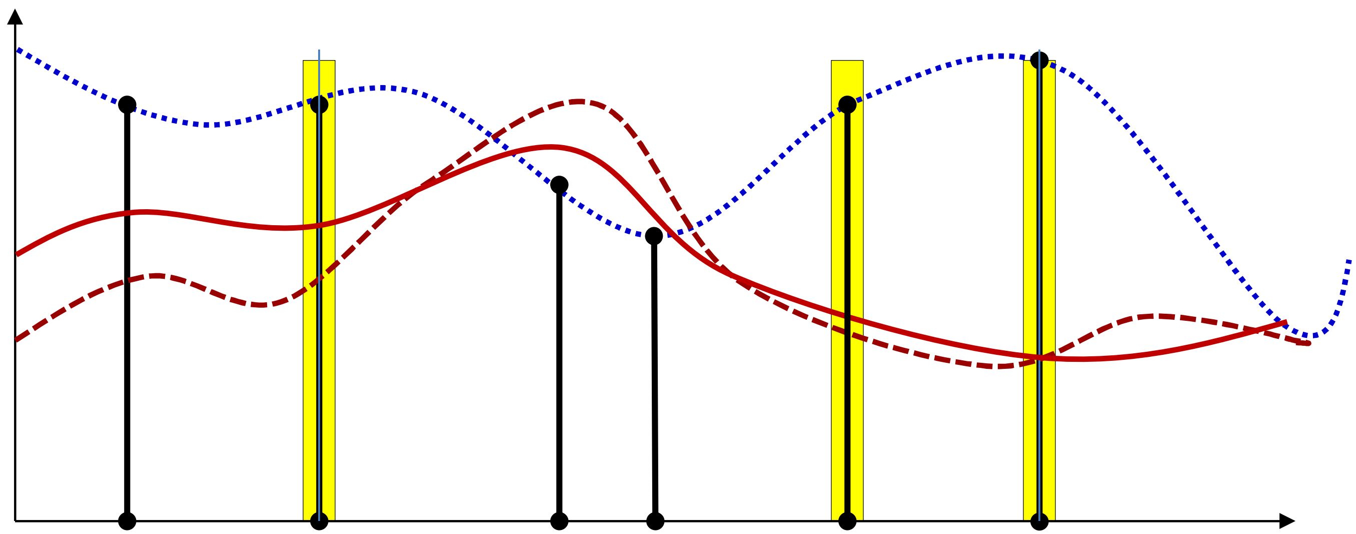
- Alternative: adjust the function at a small, randomly chosen subset of points
  - Keep adjustments small
  - If the subsets cover the training set, we will have adjusted the entire function
- As before, vary the subsets randomly in different passes through the training data

Alternative: Mini-batch update



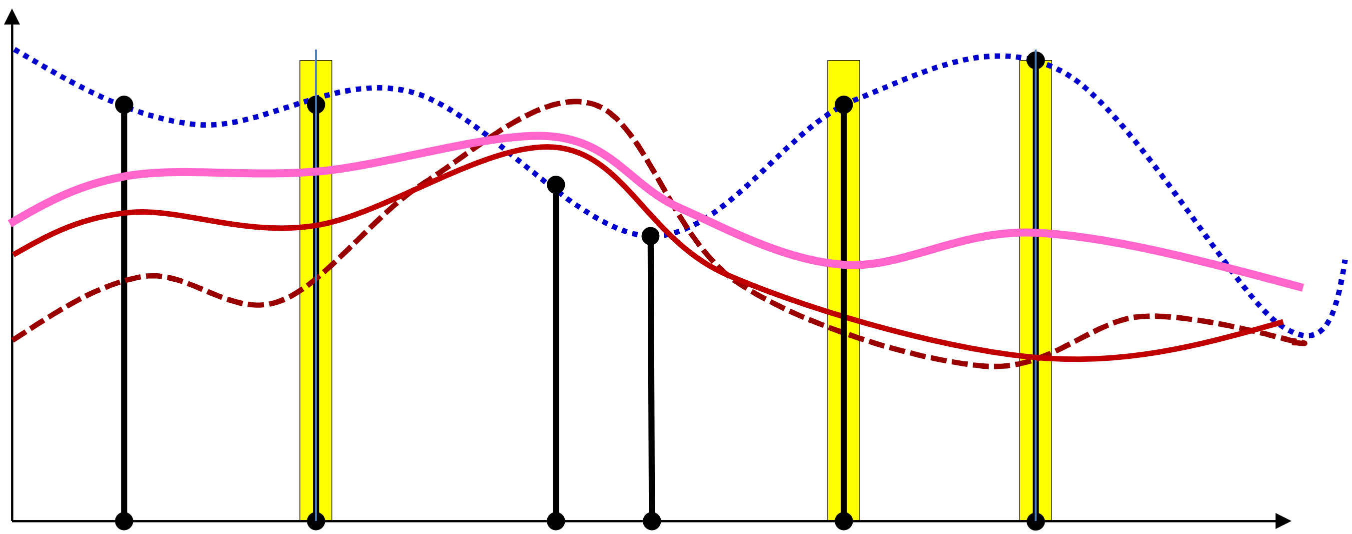
- Alternative: adjust the function at a small, randomly chosen subset of points
  - Keep adjustments small
  - If the subsets cover the training set, we will have adjusted the entire function
- As before, vary the subsets randomly in different passes through the training data

Alternative: Mini-batch update



- 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



- 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

Incremental Update: Mini-batch update

- Given (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$
- 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:
      - $\Delta W_k = 0$
    - 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

- 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:

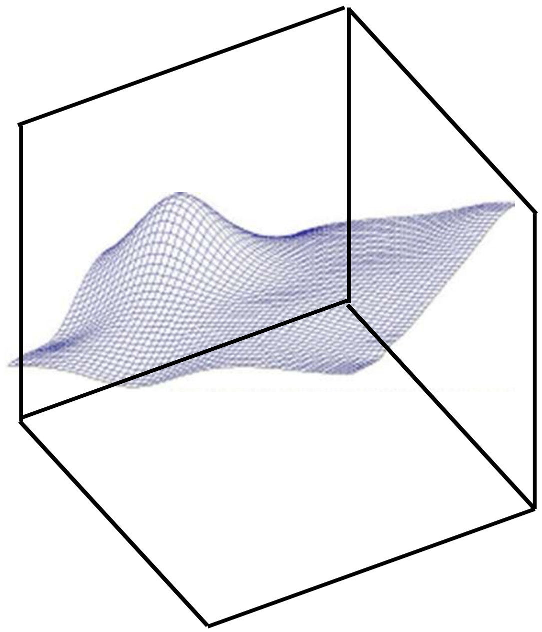
$$W_k = W_k - \eta_j \Delta W_k$$

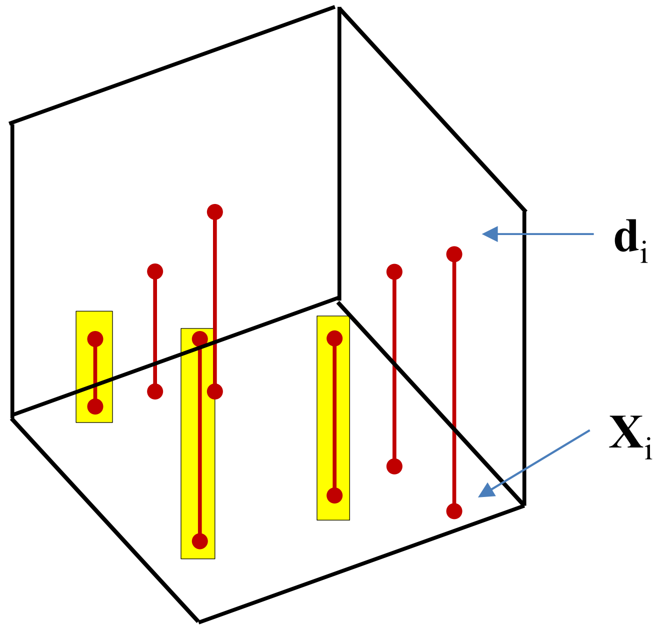
- Until Err has converged

Mini-batch size

Shrinking step size

Mini Batches





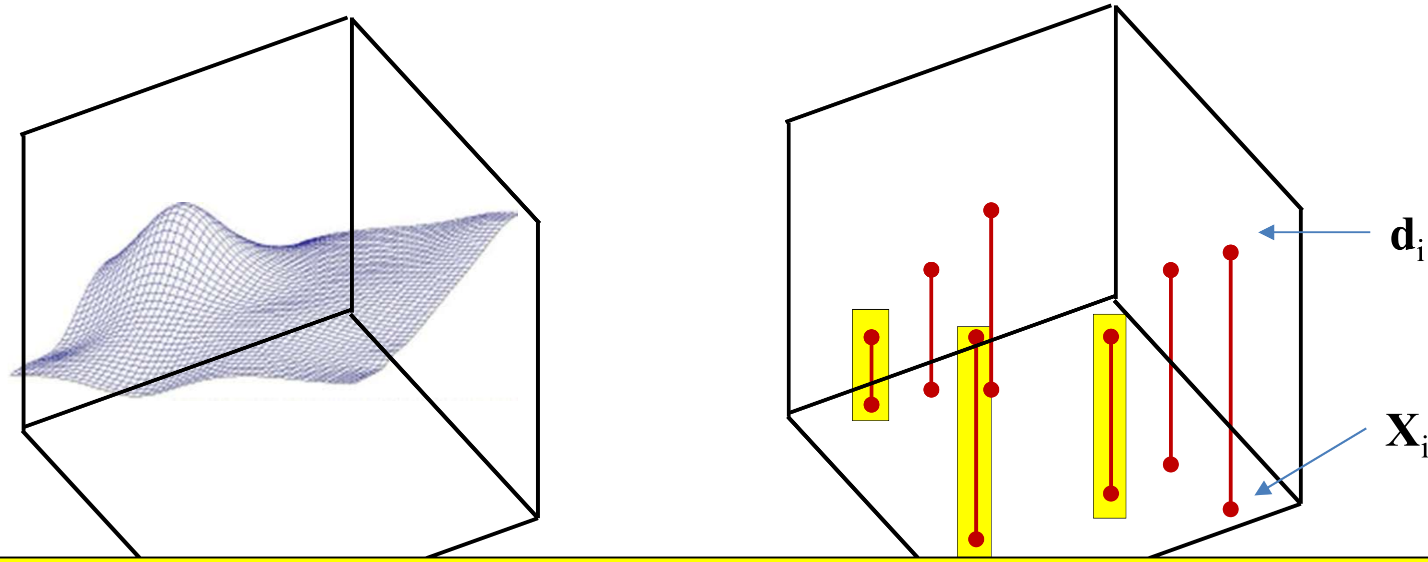
- Mini-batch updates compute and minimize a *batch loss*

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

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

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

Mini Batches



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

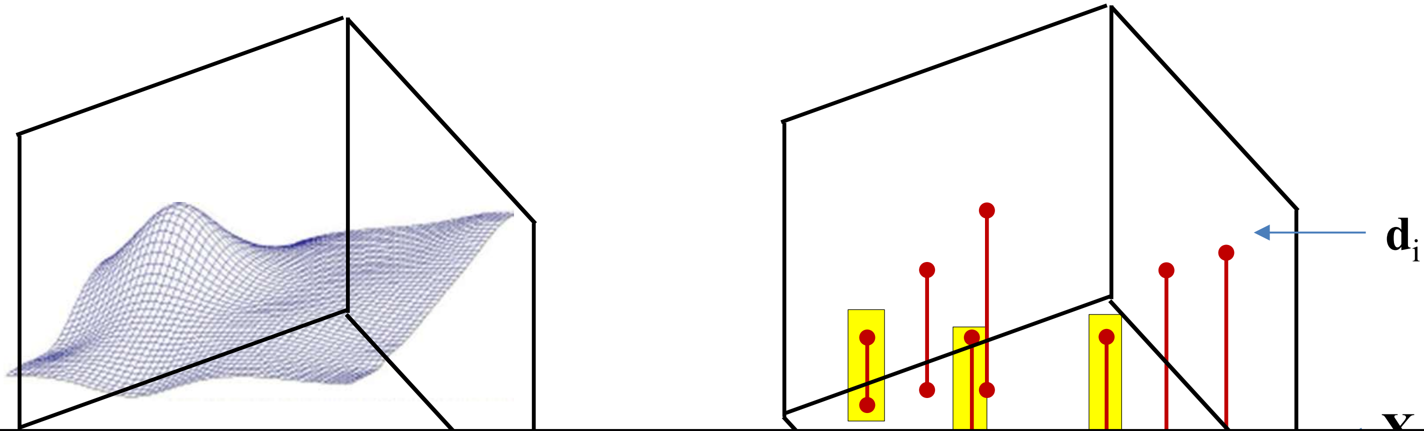
- Mini-batch updates compute and minimize a *batch loss*

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

- 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 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

- 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*

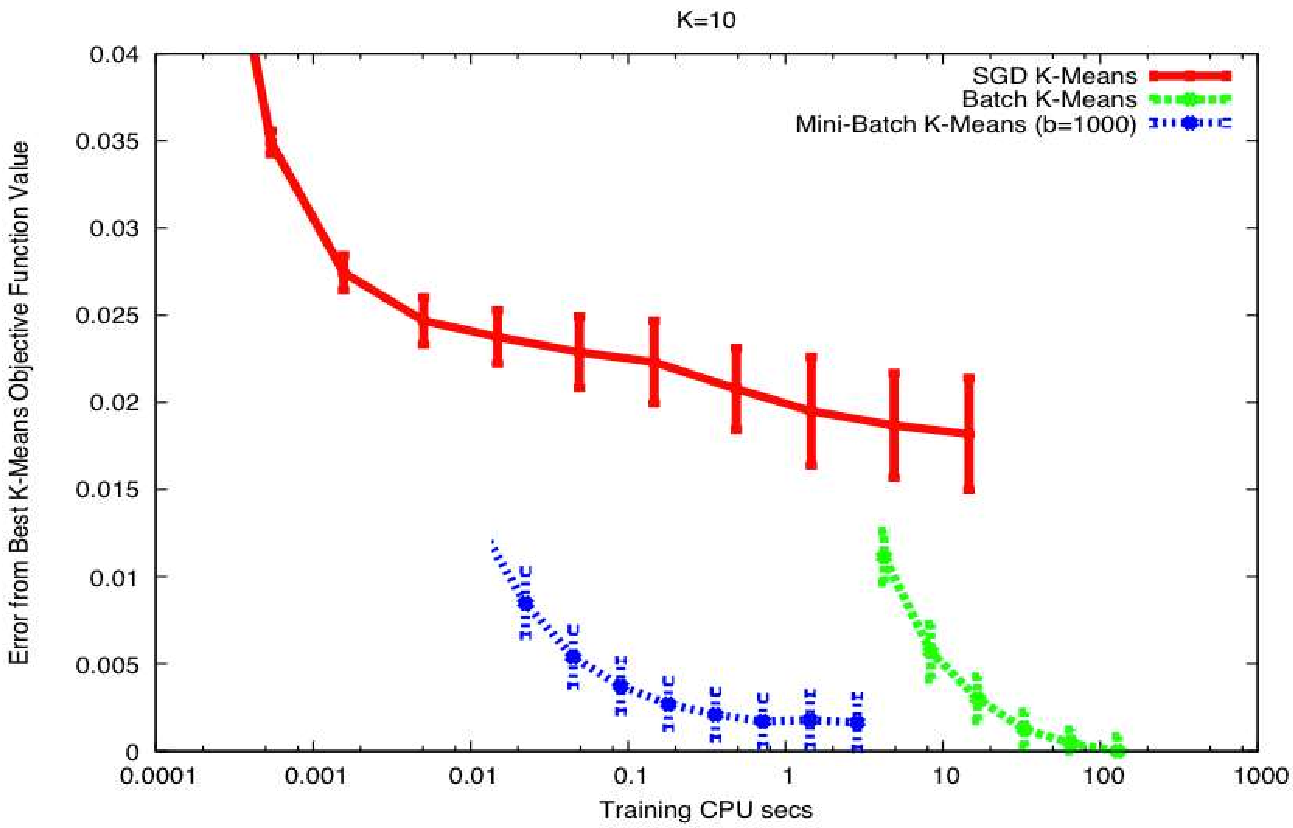
$$E[MiniBatchLoss(W)] = E\left[div\left(f(X; W), g(X)\right)\right]$$

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

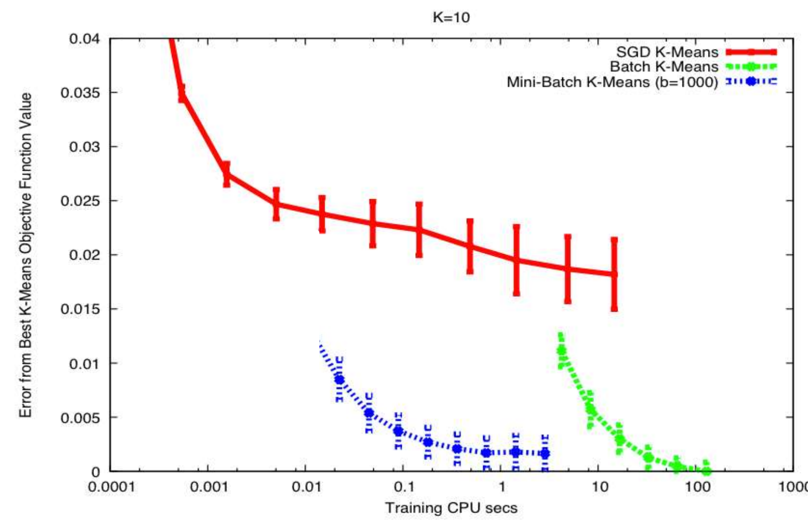
SGD example



- 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 a hyper parameter to be optimized

- 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

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

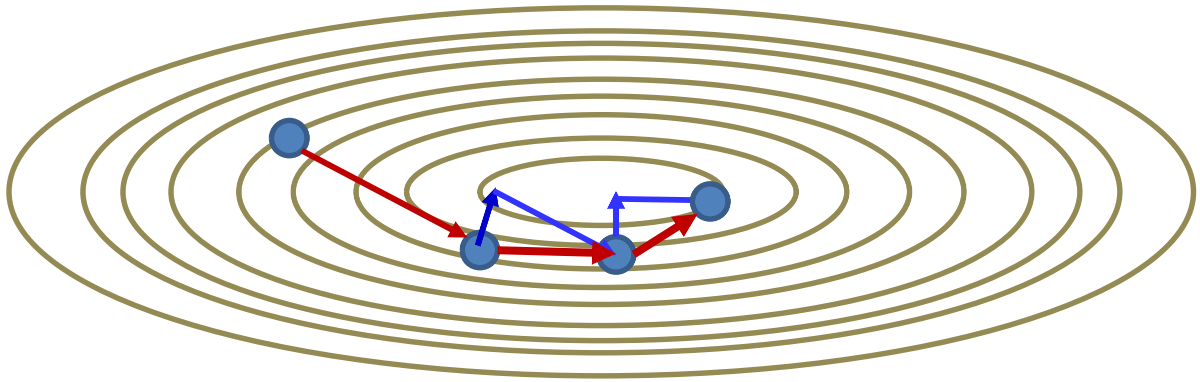
Training and minibatches

- 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

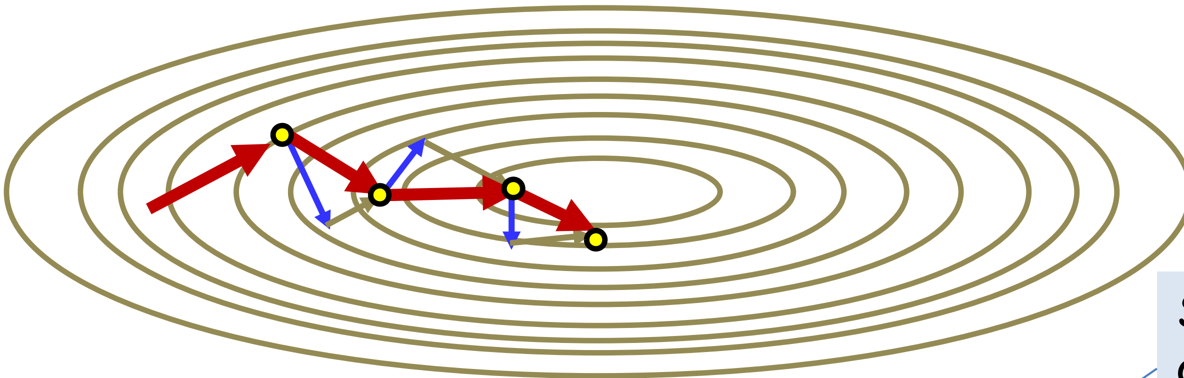


- The momentum method

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

- Updates using a running average of the gradient

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

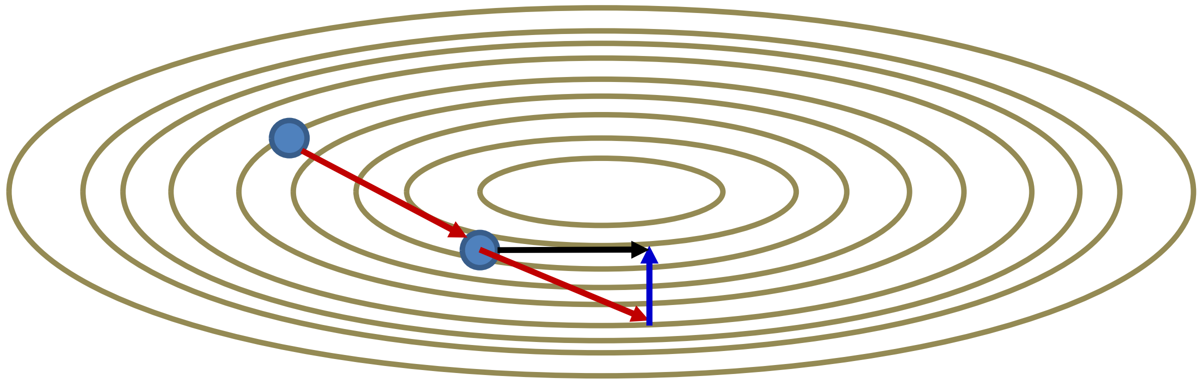
- Given (X_1, d_1), (X_2, d_2),..., (X_T, d_T)
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$, $\Delta W_k = 0$
- Do:
  - Randomly permute (X_1, d_1), (X_2, d_2),..., (X_T, d_T)
  - For $t = 1:b:T$
    - $j = j + 1$
    - For every layer k:
      - $\nabla_{W_k} Loss = 0$
    - For t' = t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

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

$$W_k = W_k + \Delta W_k$$

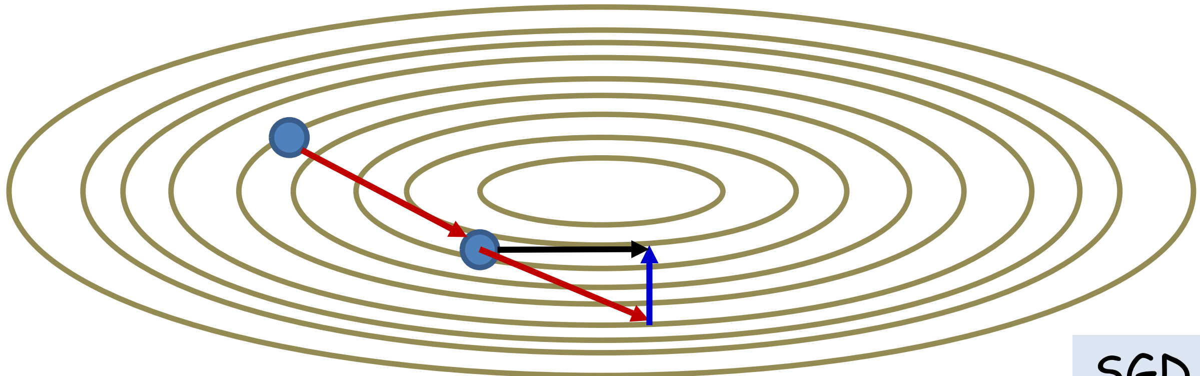
- Until $Loss$ has converged

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

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

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

Nestorov: 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:
      - $W_k = W_k + \beta \Delta W_k$
      - $\nabla_{W_k} Loss = 0$
    - 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:

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

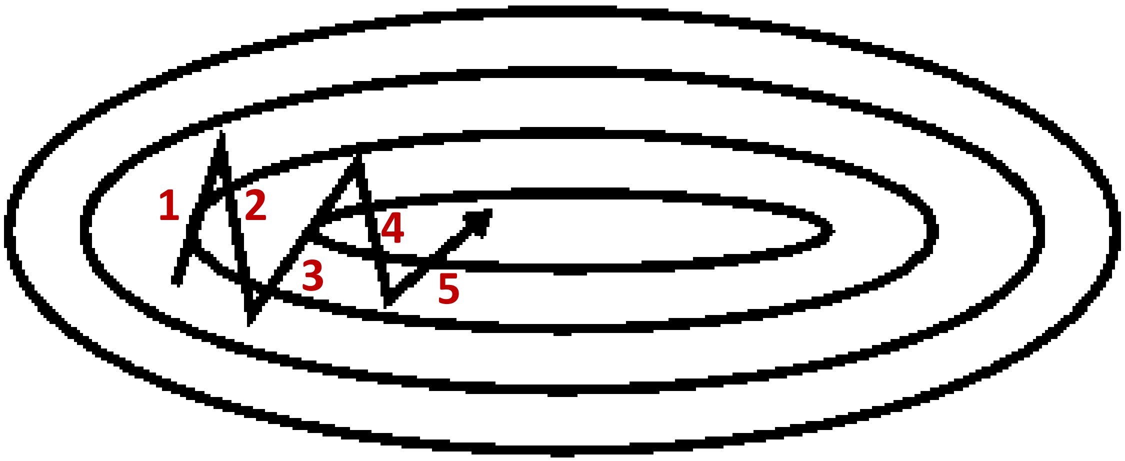
$$\Delta W_k = \beta \Delta W_k - \eta_j \nabla_{W_k} Loss^T$$

- Until $Loss$ has converged

Still higher-order methods

- Momentum and Nestorov's method improve convergence by normalizing the *mean* of the derivatives
- More recent methods take this one step further by also considering their variance
  - RMS Prop
  - Adagrad
  - AdaDelta
  - ADAM: very popular in practice
  - …
- All roughly equivalent in performance

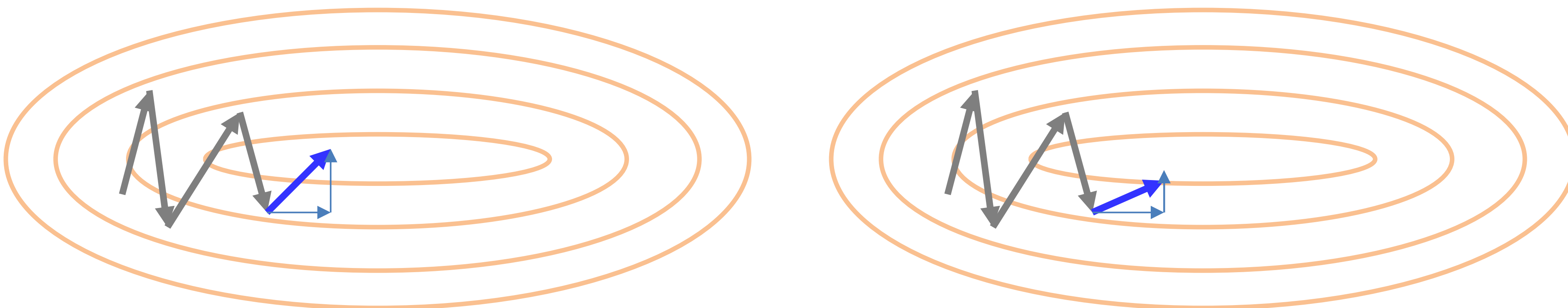
Smoothing the trajectory



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
  - Can happen even when momentum or Nestorov are used
- Improvement: Dampen step size in directions with high motion
  - ***Second order term***

Normalizing steps by second moment



- Modify usual gradient-based update:
  - Scale updates in every component in inverse proportion to the total movement of that component in recent past
    - *According to their variation (not just their average)*
- This will change the relative update sizes for the individual components
  - In the above example it would scale *down* Y component
  - And scale *up* X component (in comparison)
- We will see two popular methods that embody this principle…

RMS Prop

- Notation:
  - Updates 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 updates with large mean squared derivatives
  - scale up updates 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 update of the parameter by the *inverse* of the *root mean squared* derivative

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

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

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 update of the parameter by the *inverse* of the *root mean squared* derivative

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

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

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

ADAM: RMSprop with momentum

- RMS prop only considers a second-moment normalized version of the current gradient
- ADAM utilizes a smoothed version of the *momentum-augmented* gradient
  - Considers both first and second moments

- **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

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

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

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

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

ADAM: RMSprop with momentum

- RMS prop only considers a second-moment normalized version of the current gradient
- ADAM utilizes a smoothed version of the *momentum-augmented* gradient

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

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

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

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

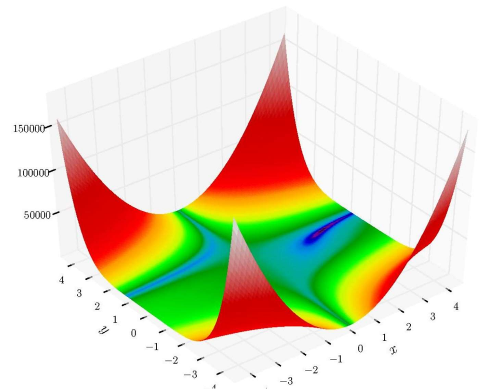
$$w_{k+1} = w_k - \frac{\eta}{\sqrt{\hat{v}_k + \epsilon}}\hat{m}_k$$

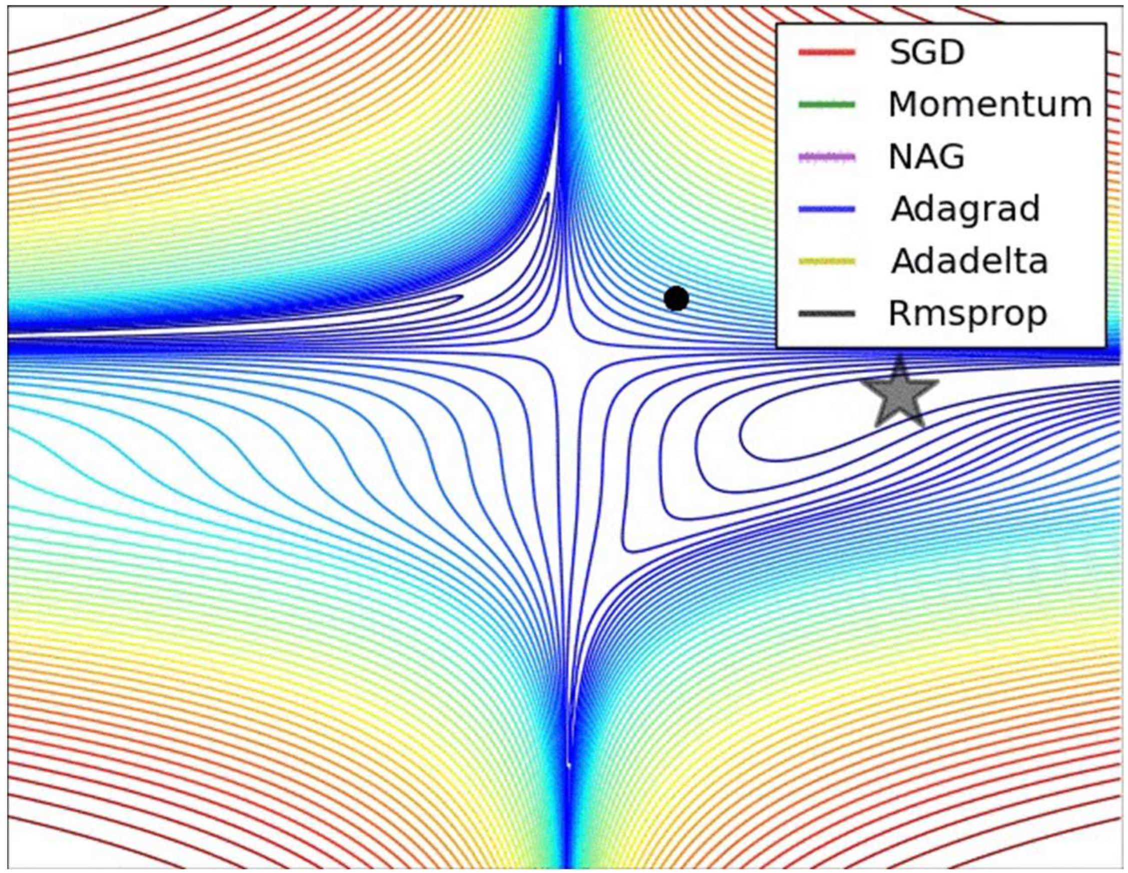
Ensures that the δ and γ terms do not dominate in early iterations

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: $\eta = 0.001, \delta = 0.9, \gamma = 0.999$

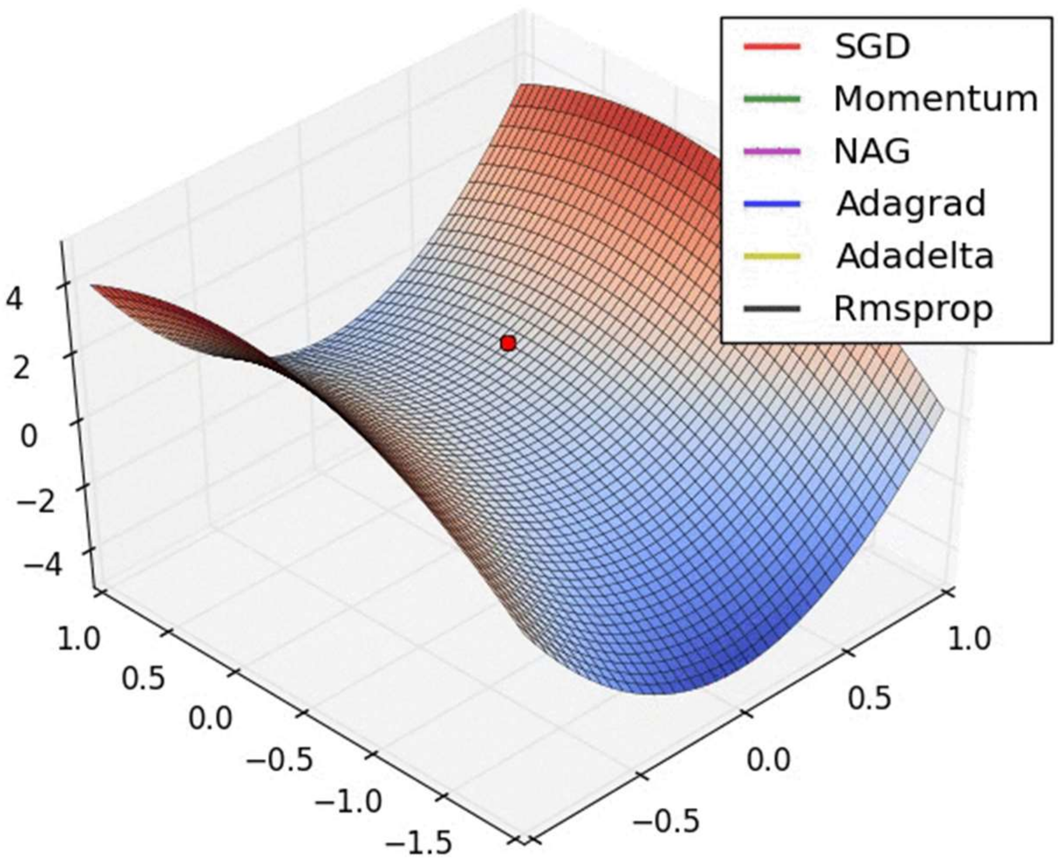
Visualizing the optimizers: Beale's Function





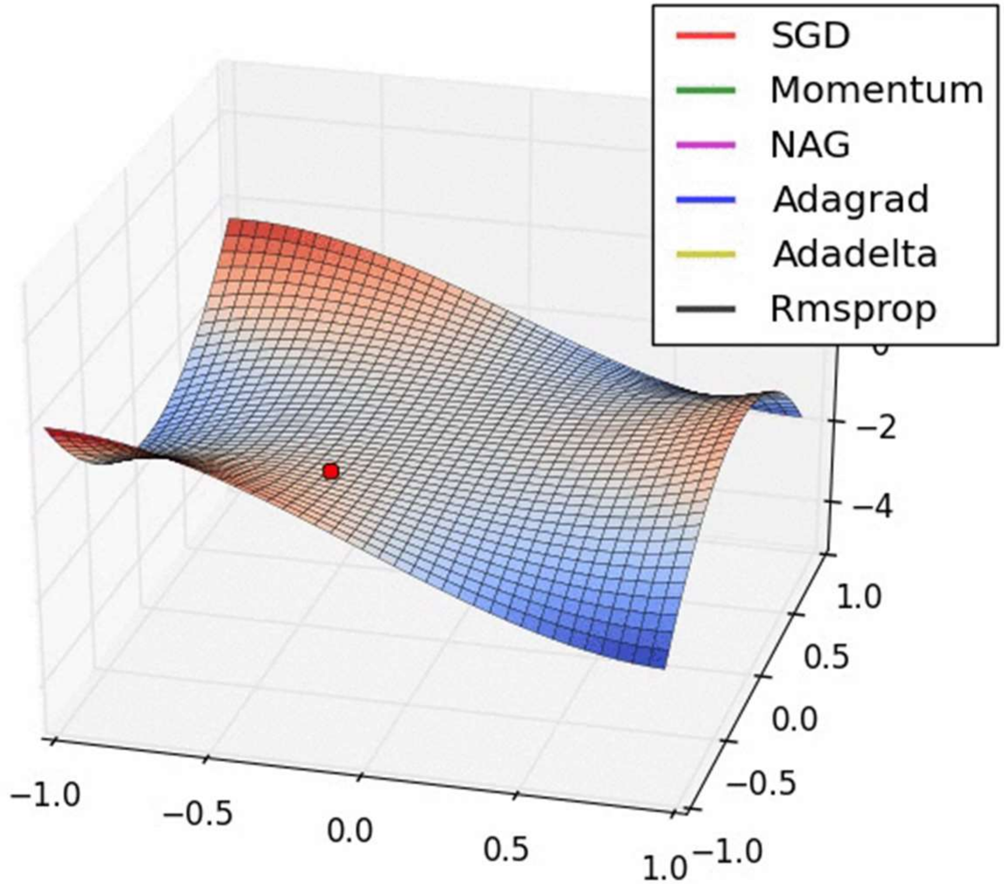
- http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

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