Training Neural Networks: Optimization

Intro to Deep Learning, Spring 2019

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

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

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

- 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

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

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

Solved through gradient descent as

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

- 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

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

Computed using backpropagation

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

Solved through gradient descent as

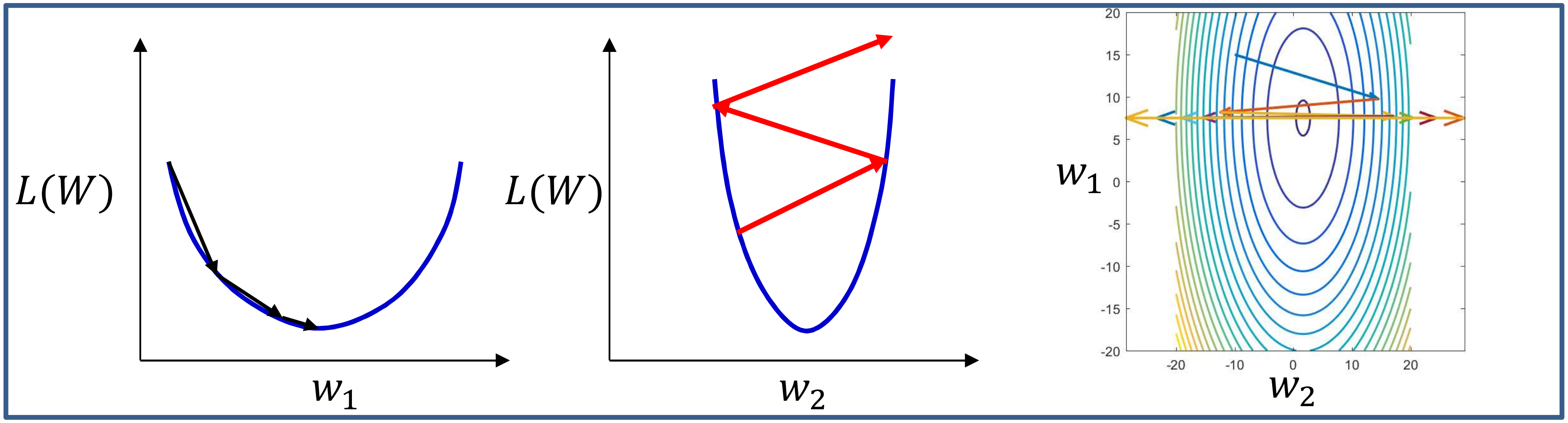
$$\widehat{W} = \arg\min_W L(W) \quad \Rightarrow \quad W_k = W_{k-1} - \eta \nabla_W L(W)^T$$

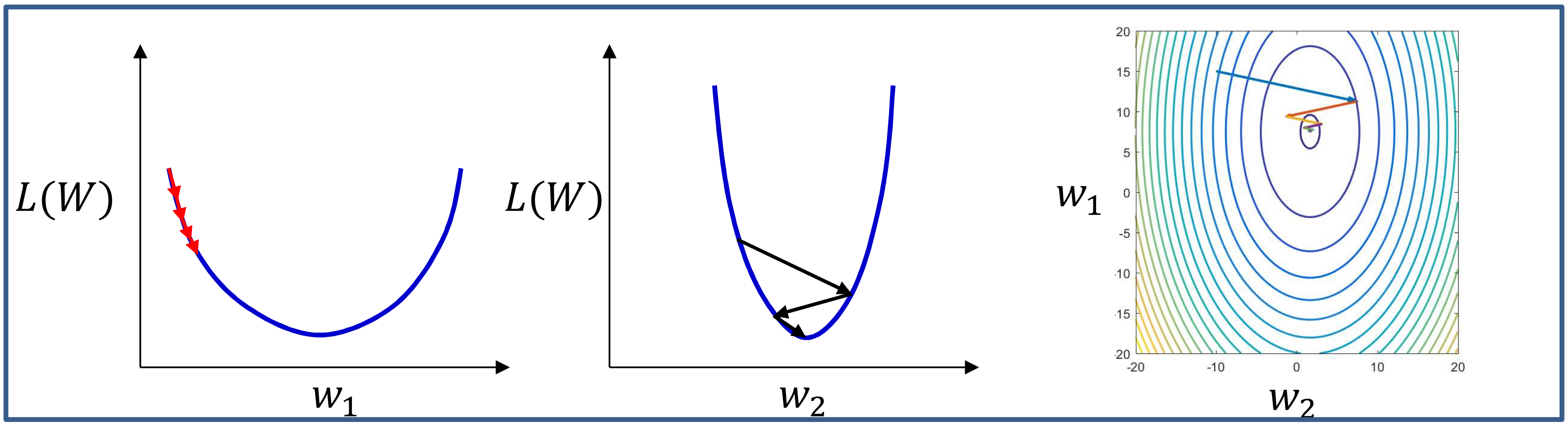
- The gradient of the total loss is the average of the gradients of the loss for the individual instances
- The gradient can be plugged into gradient descent update to learn the network parameters

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

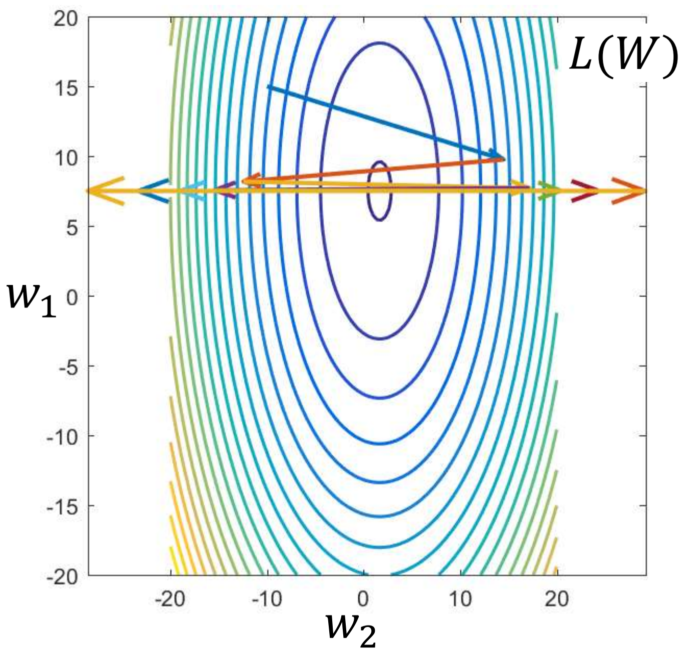


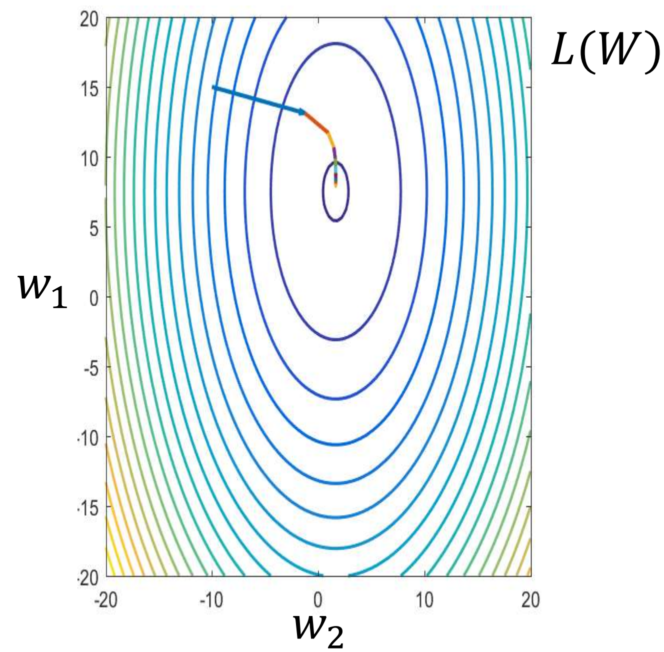


$$W_k = W_{k-1} - \eta \nabla_w L(W)^T$$

- 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

Solutions for problem with gradient descent

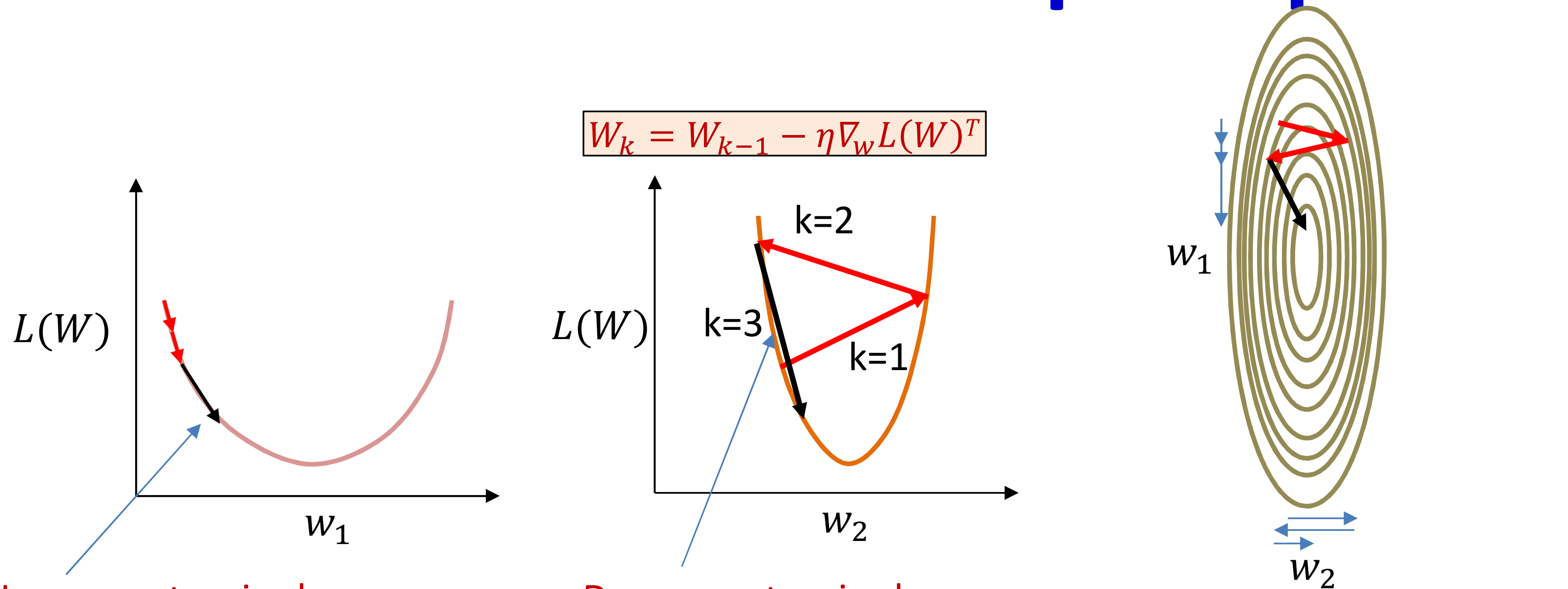
- Try to normalize curvature in all directions
  - Second order methods, e.g. Newton's method
  - Too expensive: require inversion of a giant Hessian

- Treat each dimension independently:
  - Rprop, quickprop
  - Works, but ignores dependence between dimensions
    - Can result in unexpected behavior
  - Can still be too slow

Quick Recap

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

Momentum methods: principle



Increase stepsize because previous updates consistently moved weight right

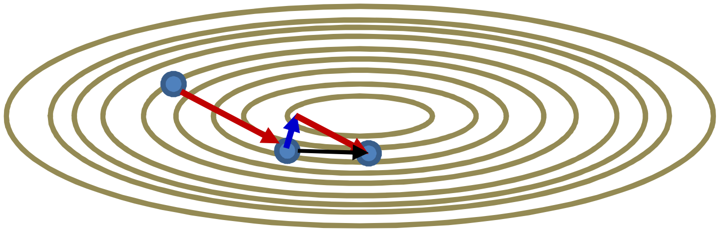
Decrease stepsize because previous updates kept changing direction

Stepsize shrinks along w2 but increases along w1

- Ideally: Have component-specific step size
  - Too many independent parameters (maintain a step size for every weight/bias)
- 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

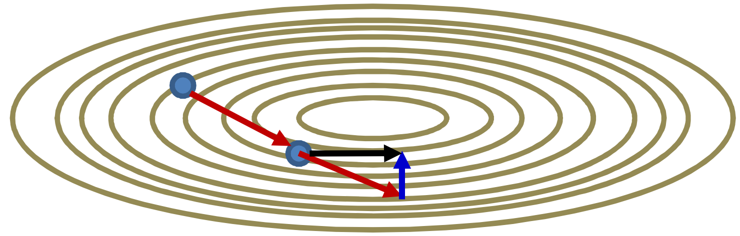
Quick recap: Momentum methods

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: Topics for the day

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

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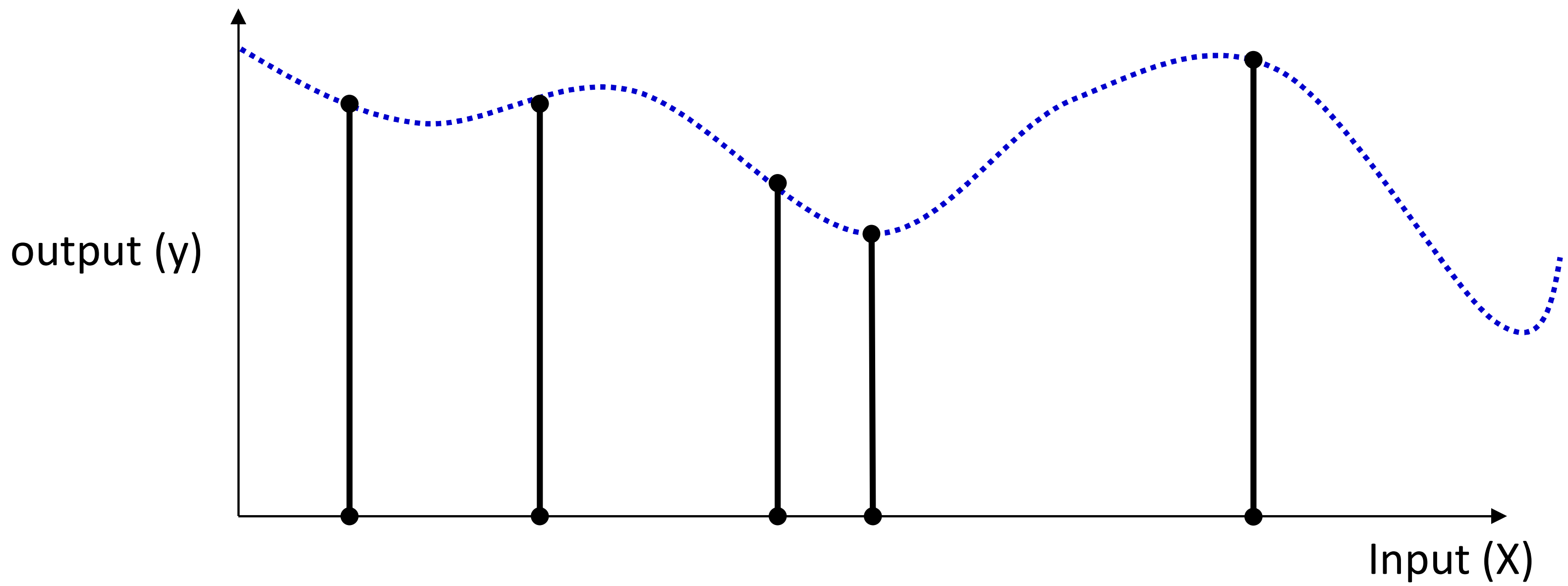
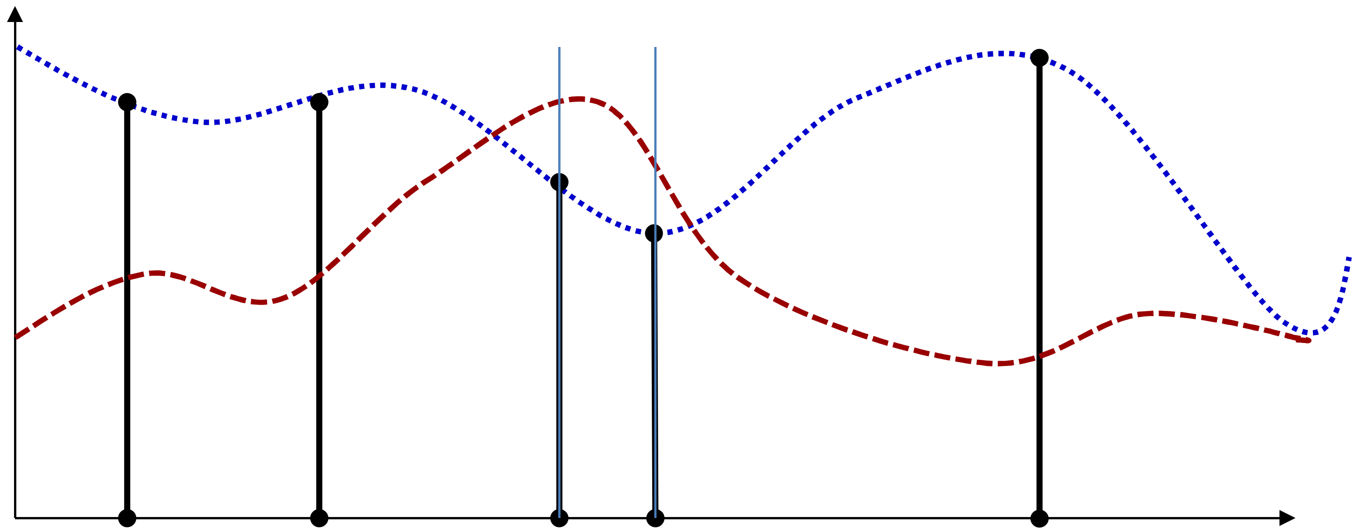
The training formulation



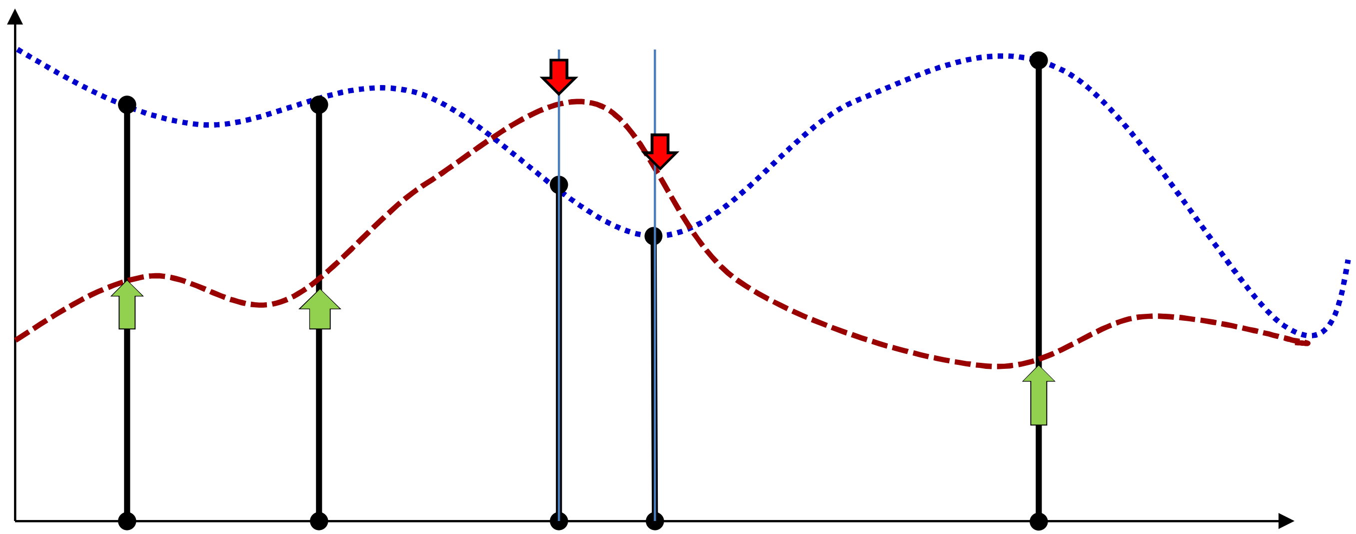
- Given input output pairs at a number of locations, estimate the entire function

Gradient descent



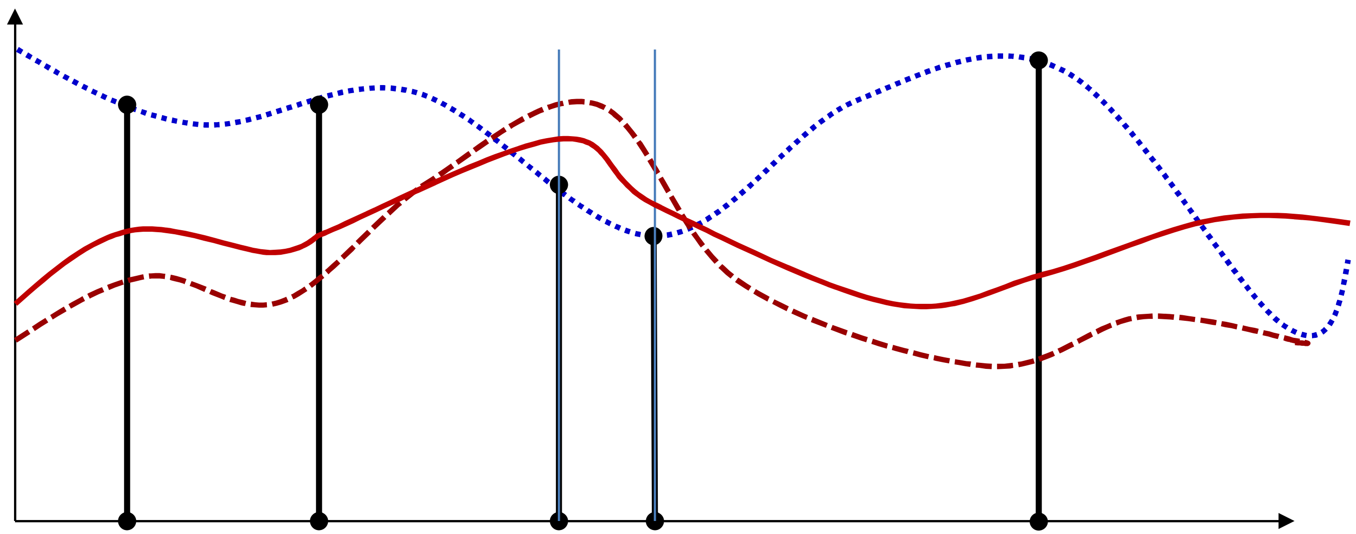
- Start with an initial function

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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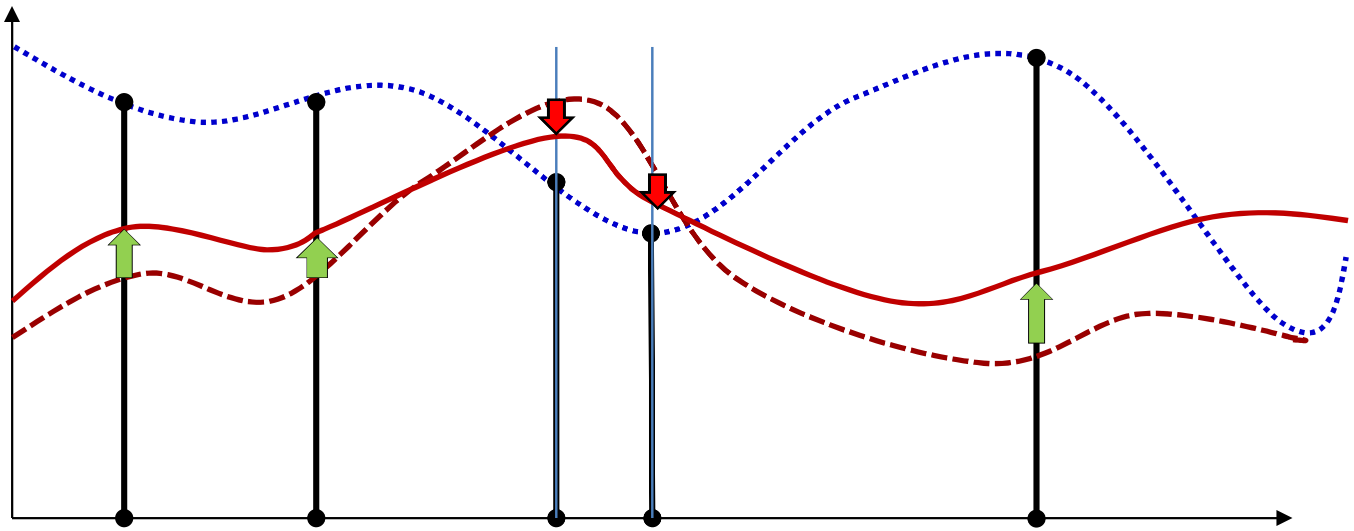

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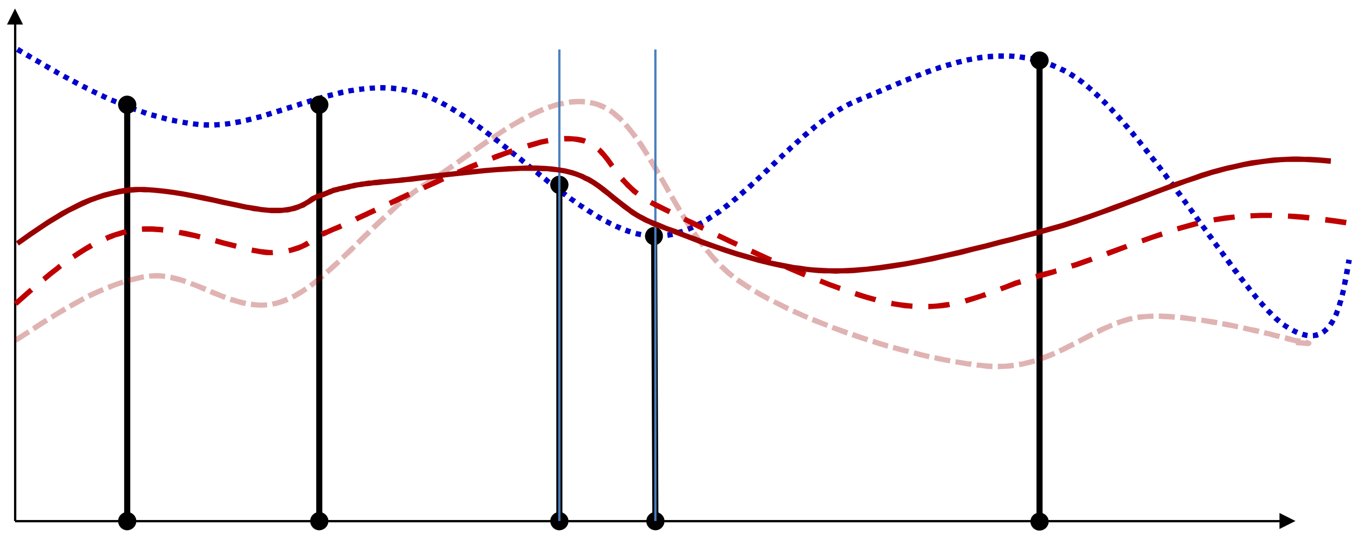

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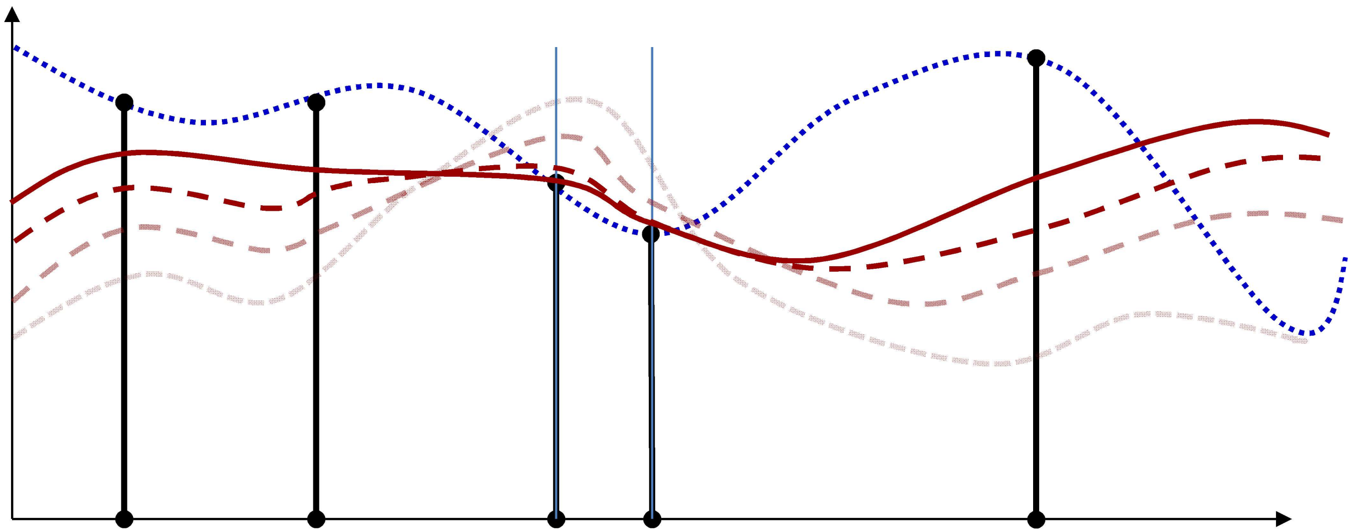

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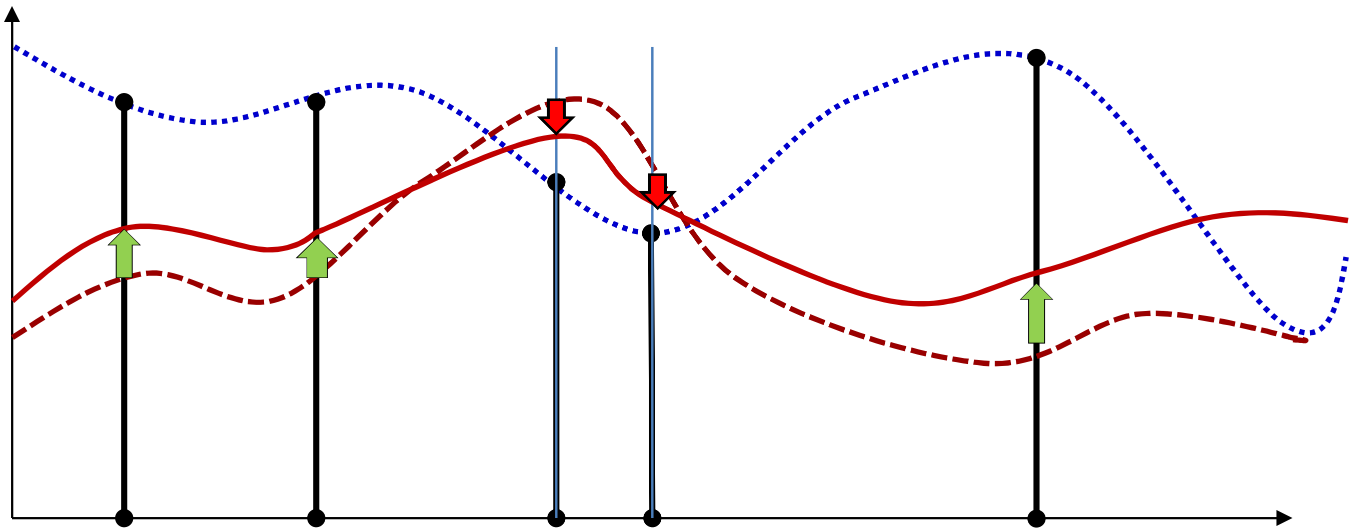
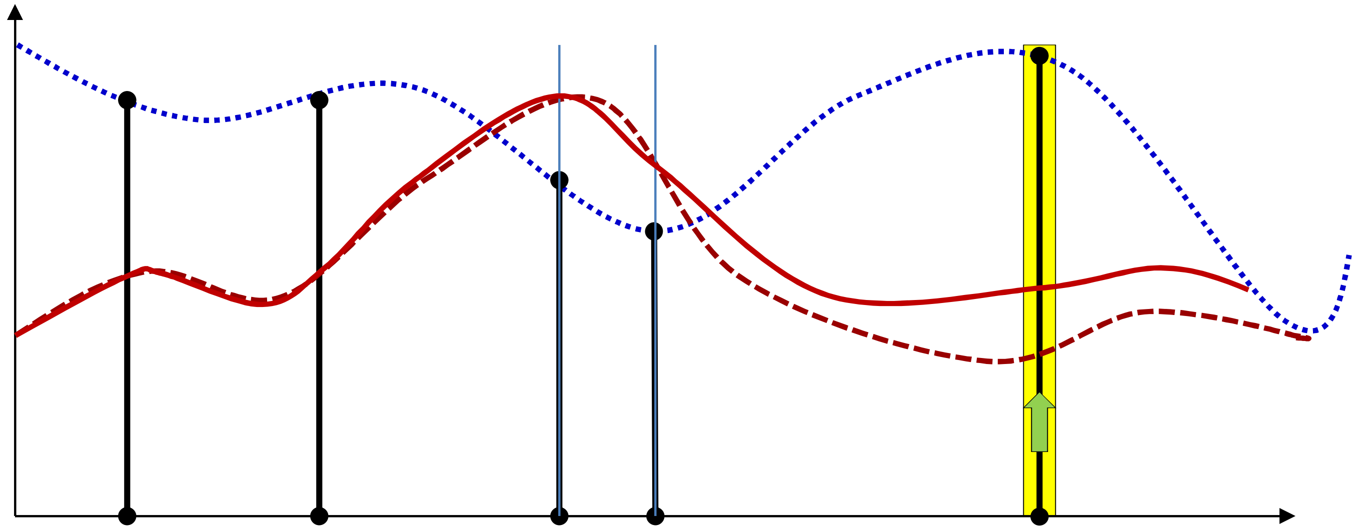
Effect of number of samples



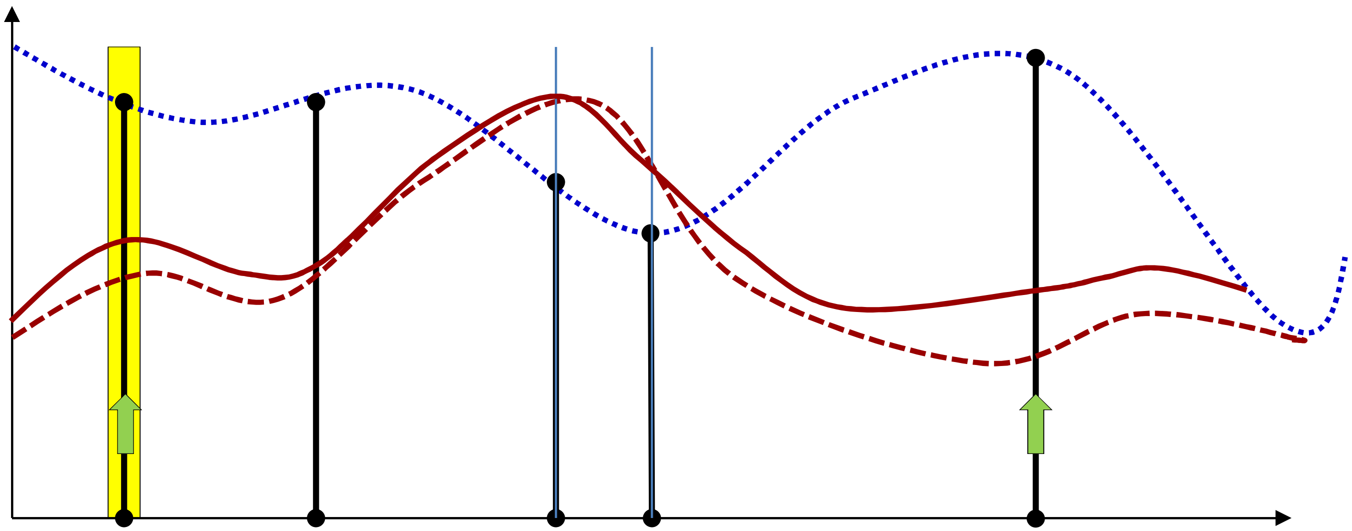
- Problem with conventional gradient descent: we try to simultaneously adjust the function at *all* training points
  - We must process *all* training points before making a single adjustment
  - “Batch” update

Alternative: Incremental update



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

Alternative: Incremental update



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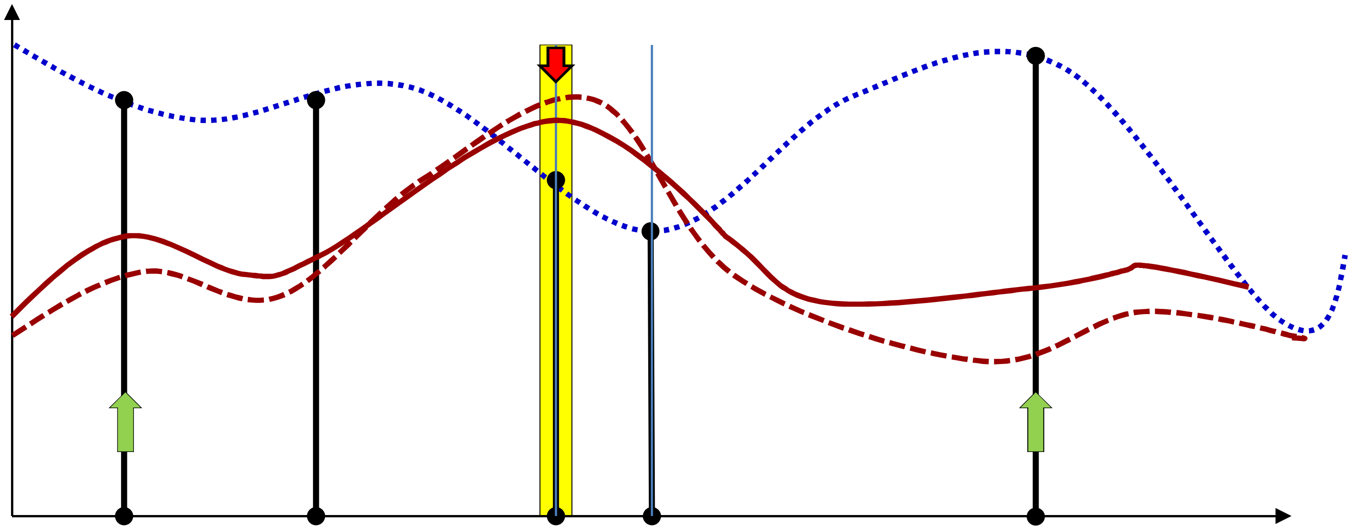

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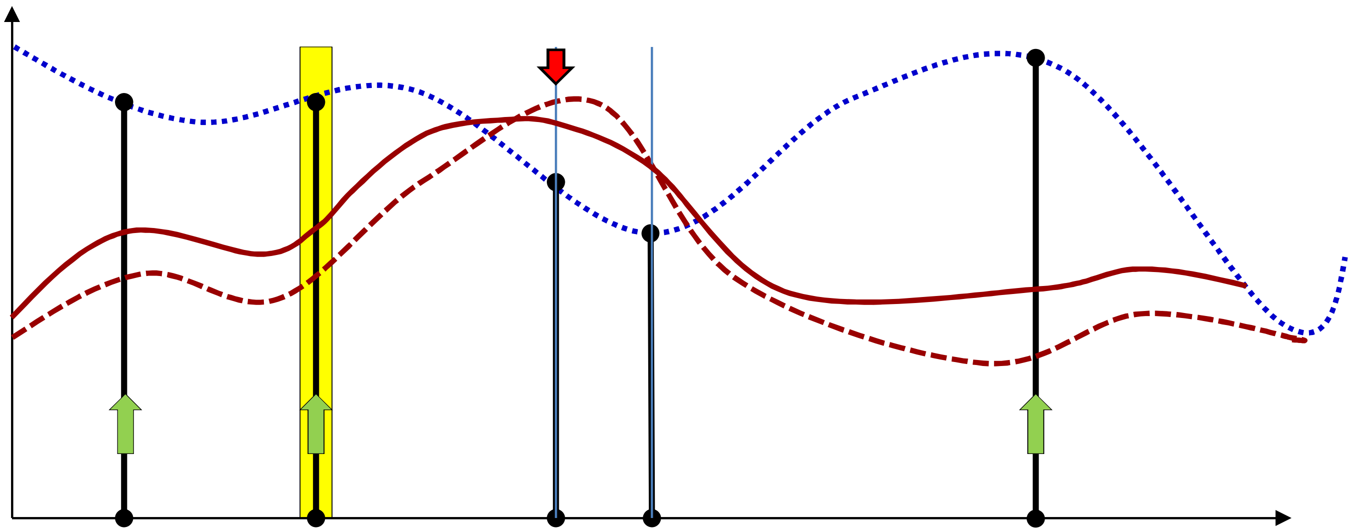

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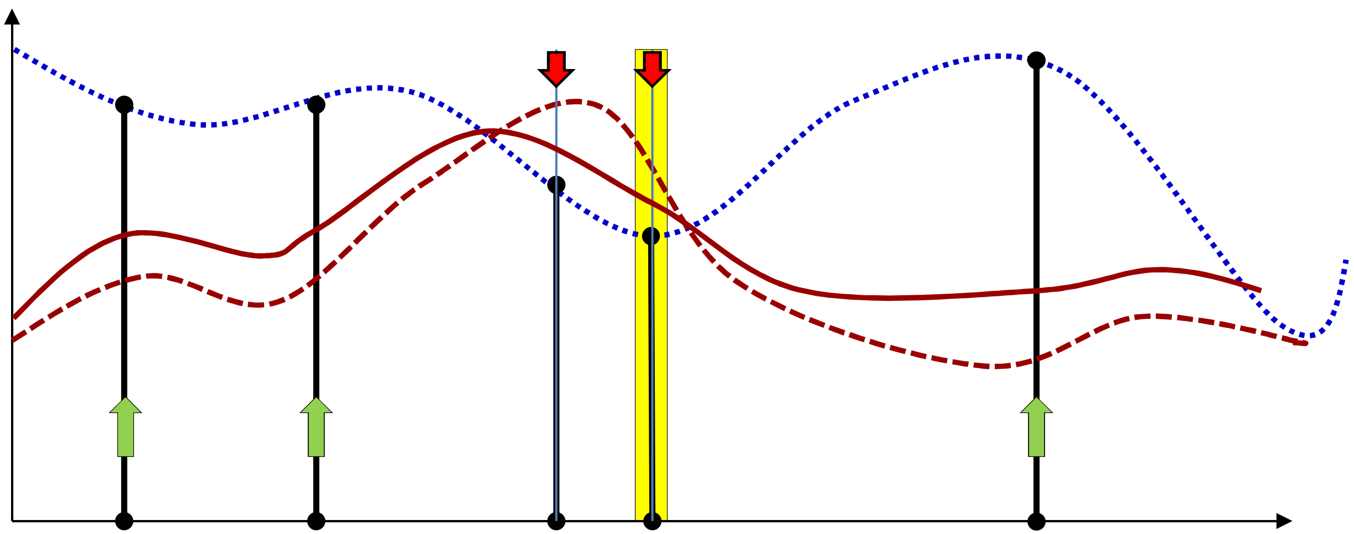


- Alternative: adjust the function at one training point at a time
  - Keep adjustments small
  - Eventually, when we have processed all the training points, we will have adjusted the entire function
    - With *greater* overall adjustment than we would if we made a single "Batch" update

Incremental Update: Stochastic Gradient Descent

- Given (X_1, d_1), (X_2, d_2),…, (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

Stochastic Gradient Descent

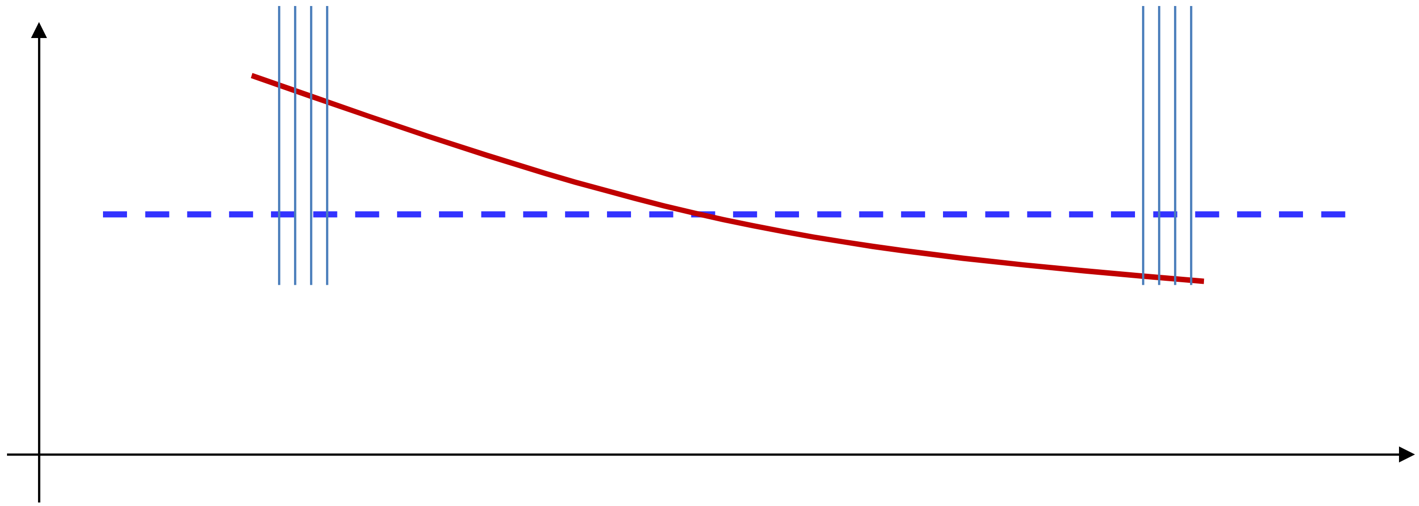
- The iterations can make multiple passes over the data
- A single pass through the entire training data is called an "epoch"
  – An epoch over a training set with T samples results in T updates of parameters

Incremental Update: 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: ← Over multiple epochs
  - For all $t = 1:T$ (One epoch)
    - 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

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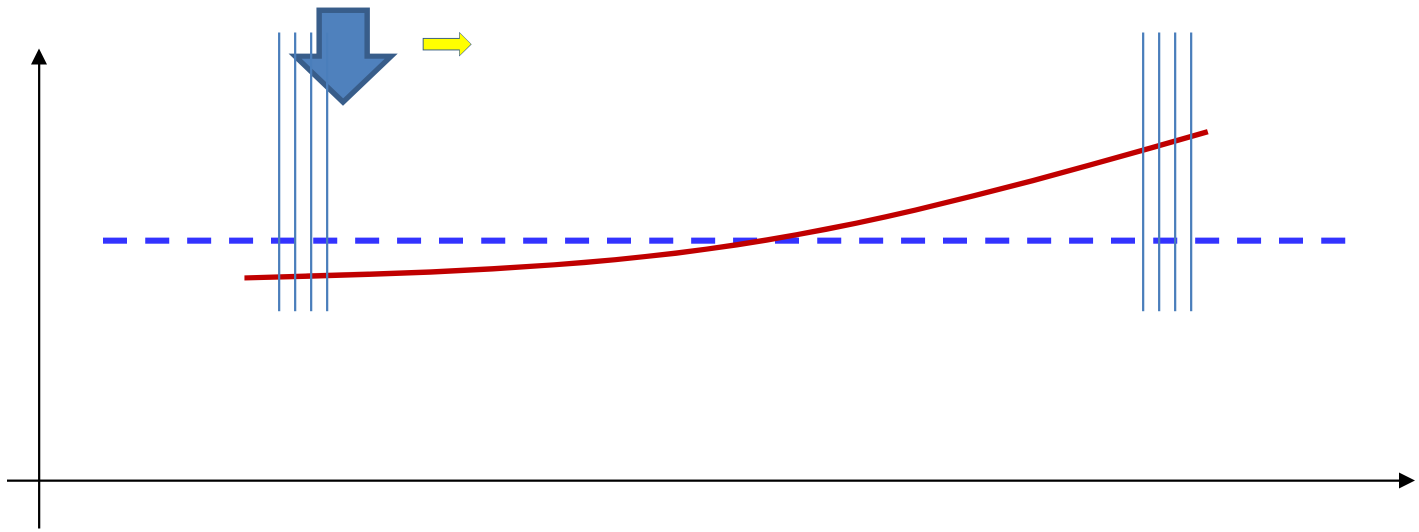

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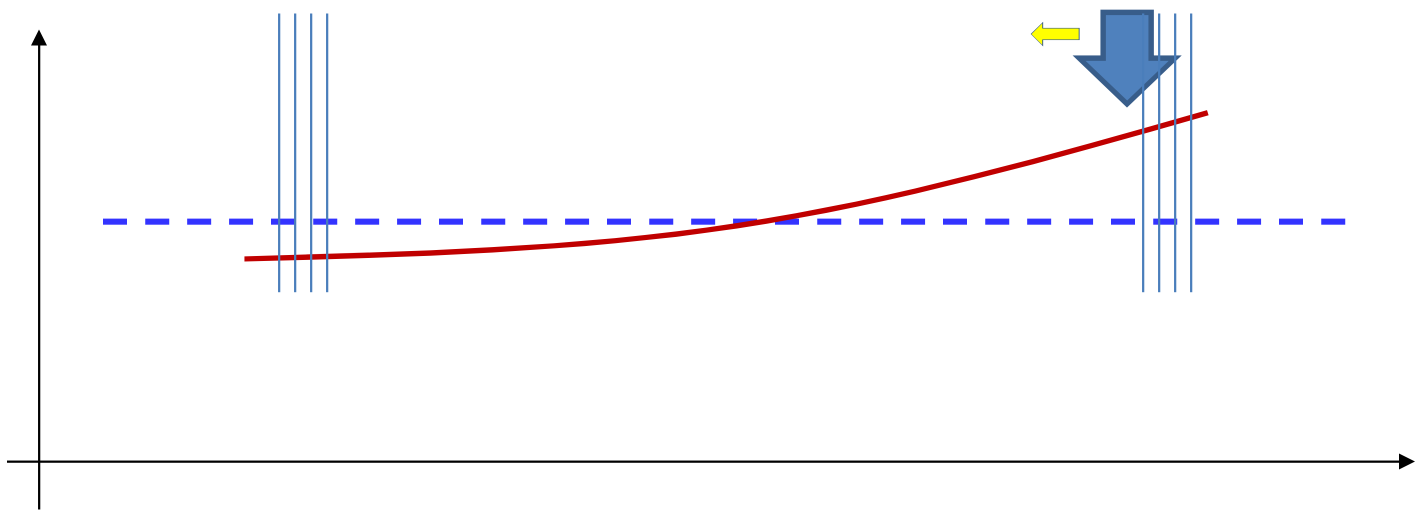

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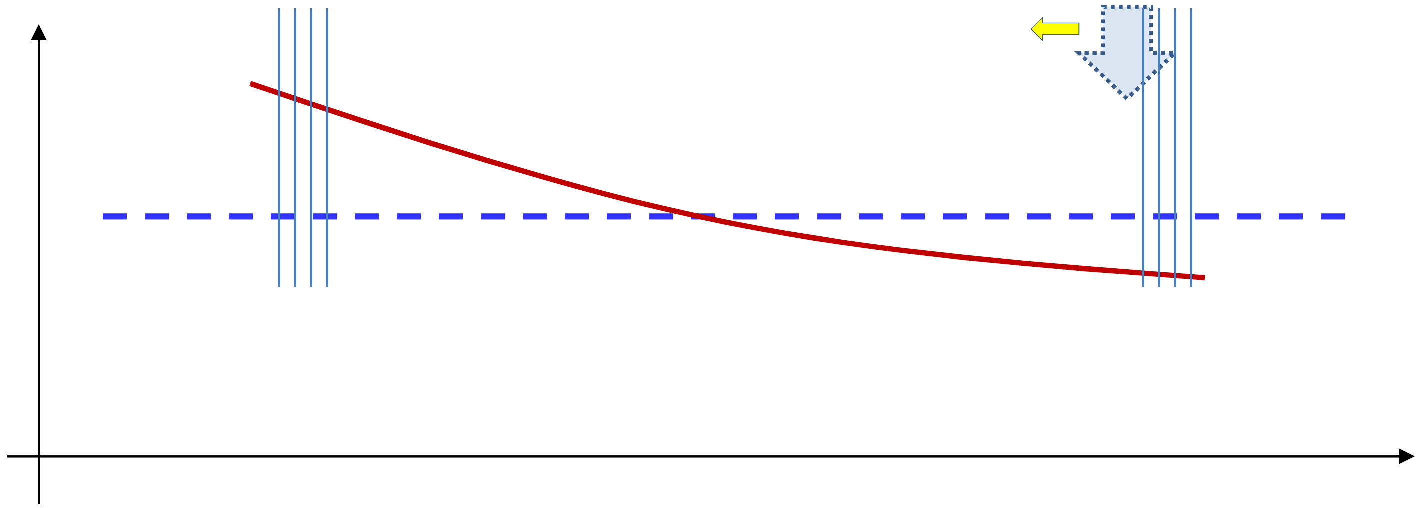

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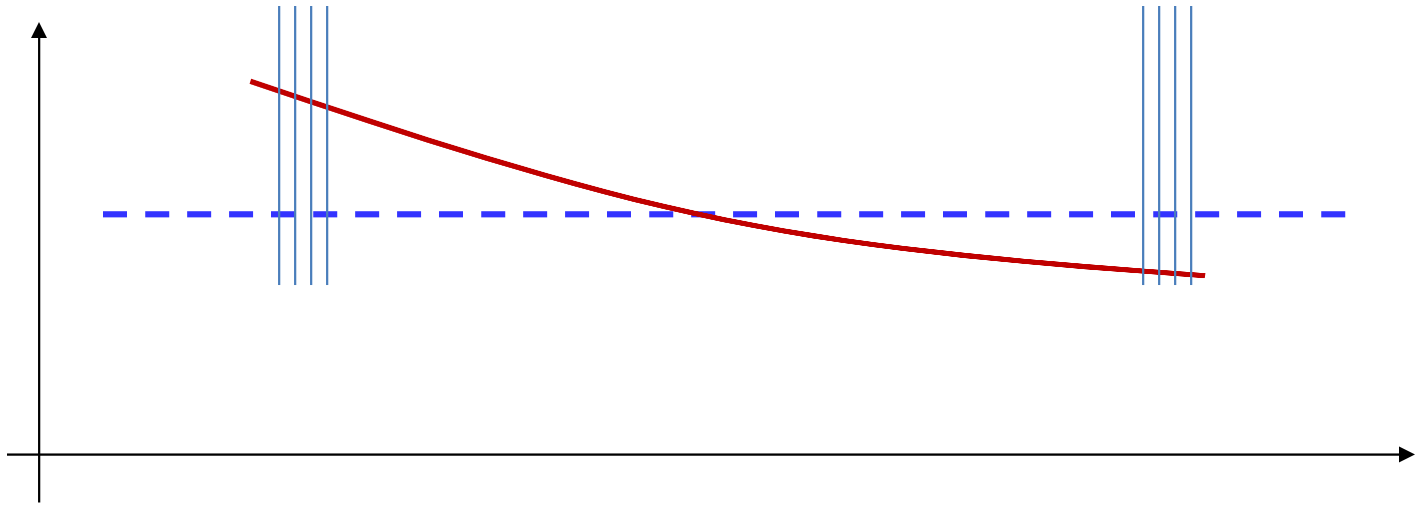

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- We must go through them *randomly* to get more convergent behavior

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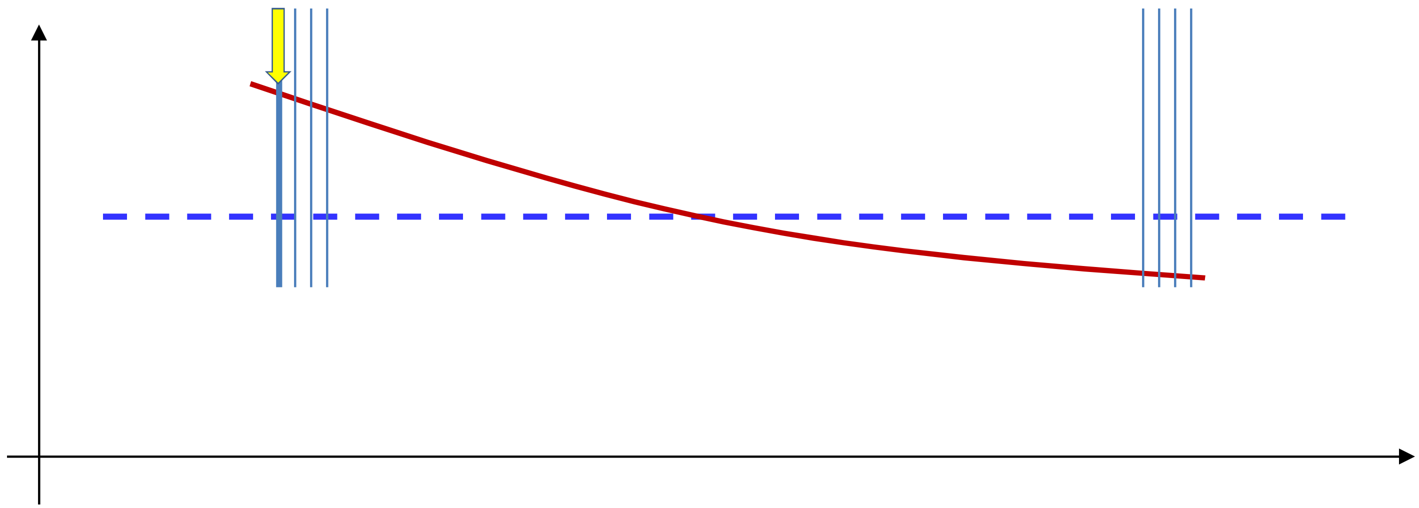

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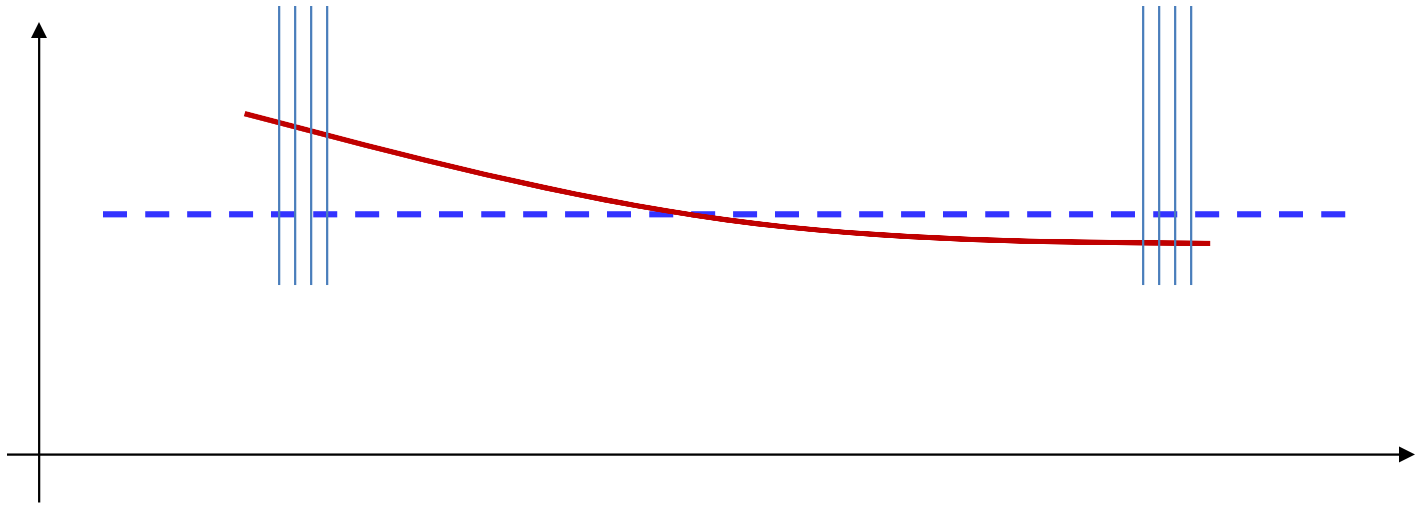

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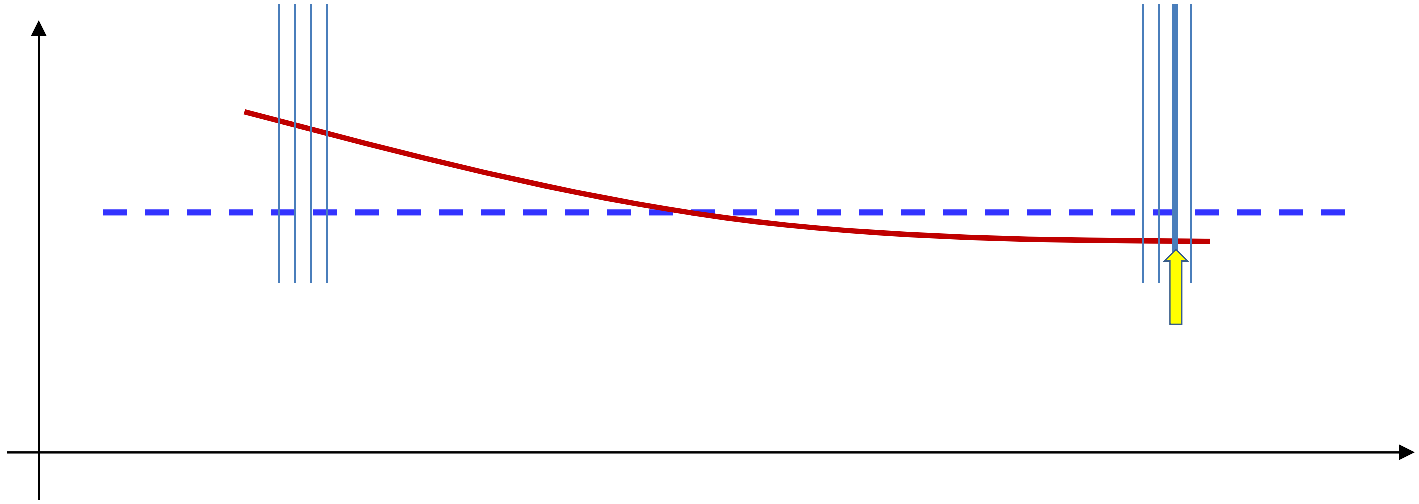

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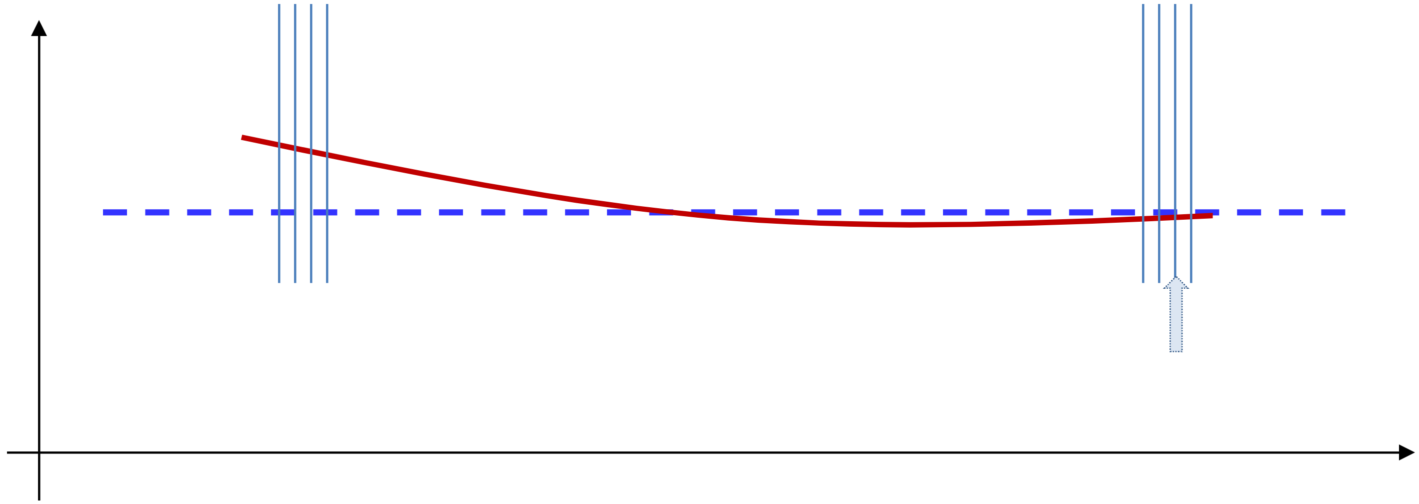

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- Initialize all weights $W_1, W_2, \ldots, W_K$
- Do:
  - Randomly permute $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
  - For all $t = 1:T$
    - For every layer k:
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$$W_k = W_k - \eta \nabla_{W_k}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

- 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

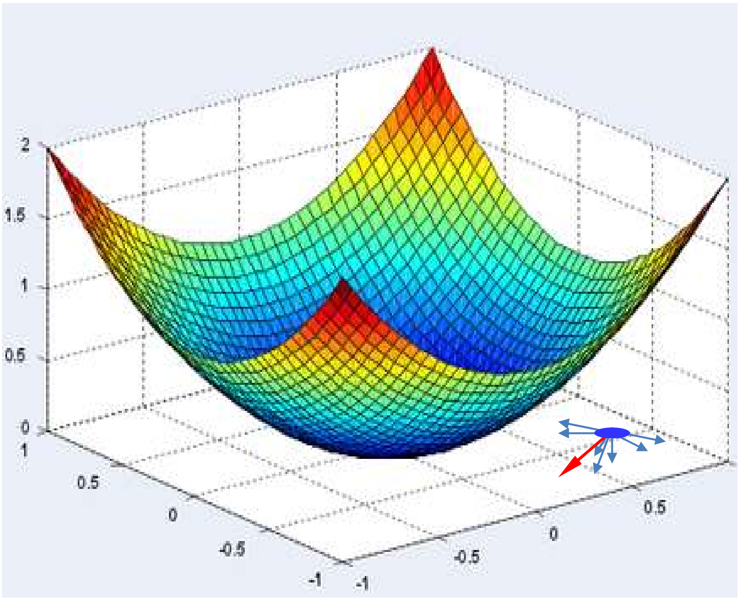
Explanations and restrictions

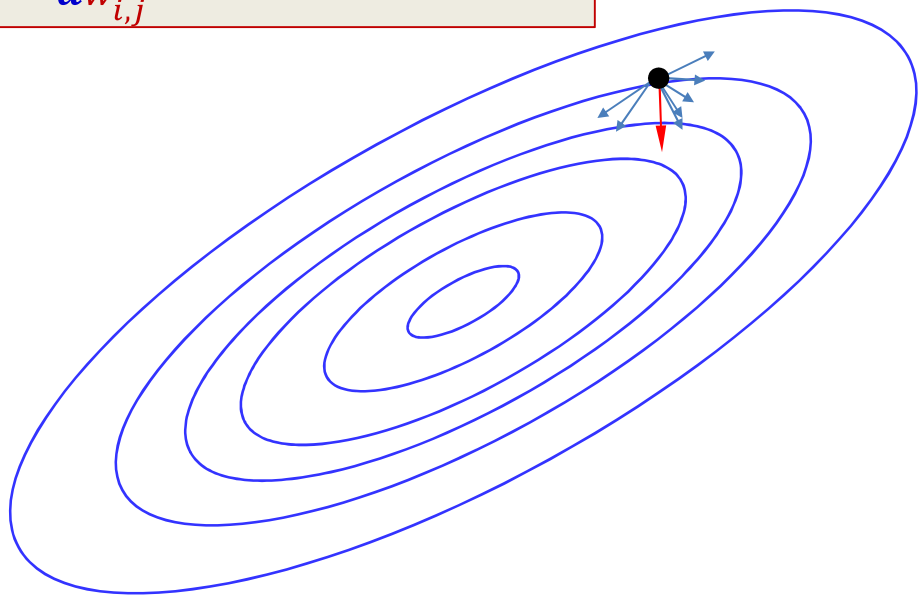
- So why does this process of incremental updates work?
- Under what conditions?

- For "why": first consider a simplistic explanation that's often given
  - Look at an extreme example

The expected behavior of the gradient

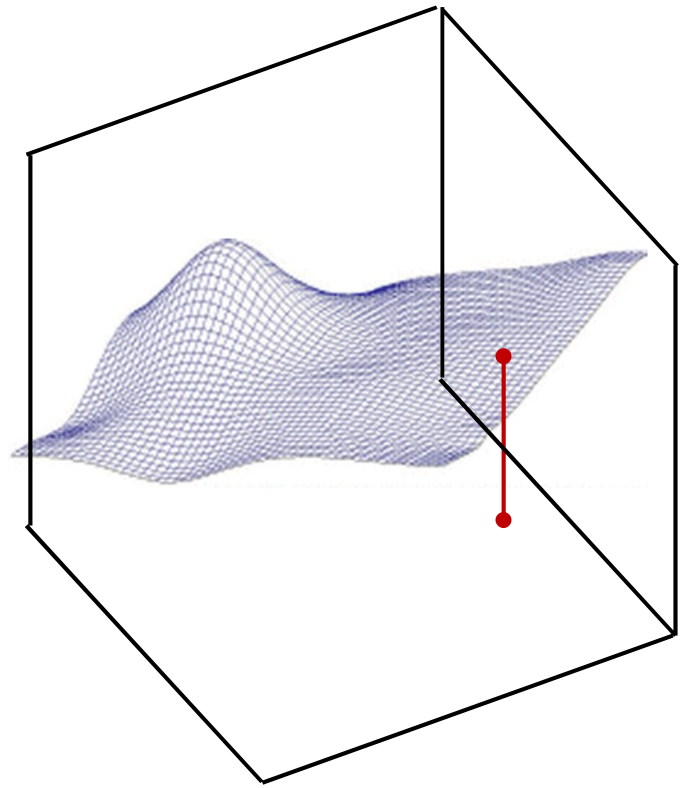
$$\frac{dE(\mathbf{W}^{(1)},\mathbf{W}^{(2)},\ldots,\mathbf{W}^{(K)})}{dw_{i,j}^{(k)}} = \frac{1}{T}\sum_i \frac{dDiv(\mathbf{Y}(\mathbf{X}_i),\mathbf{d}_i;\mathbf{W}^{(1)},\mathbf{W}^{(2)},\ldots,\mathbf{W}^{(K)})}{dw_{i,j}^{(k)}}$$





- 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

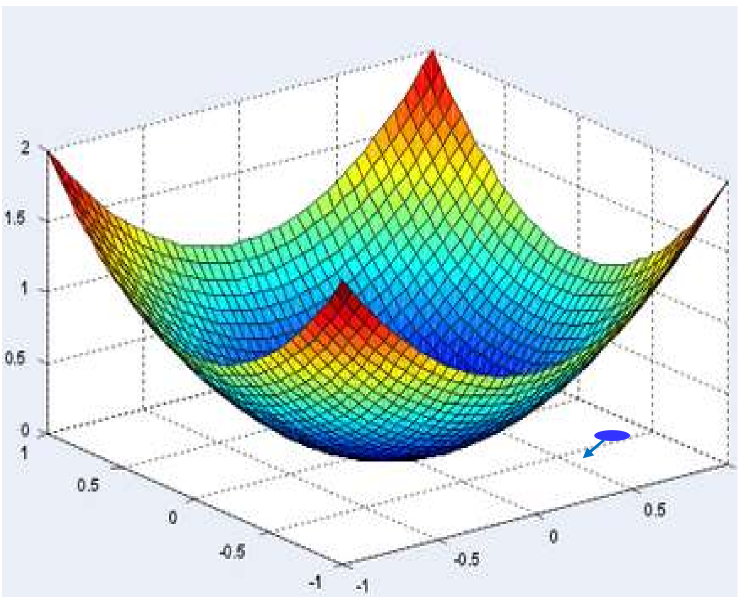


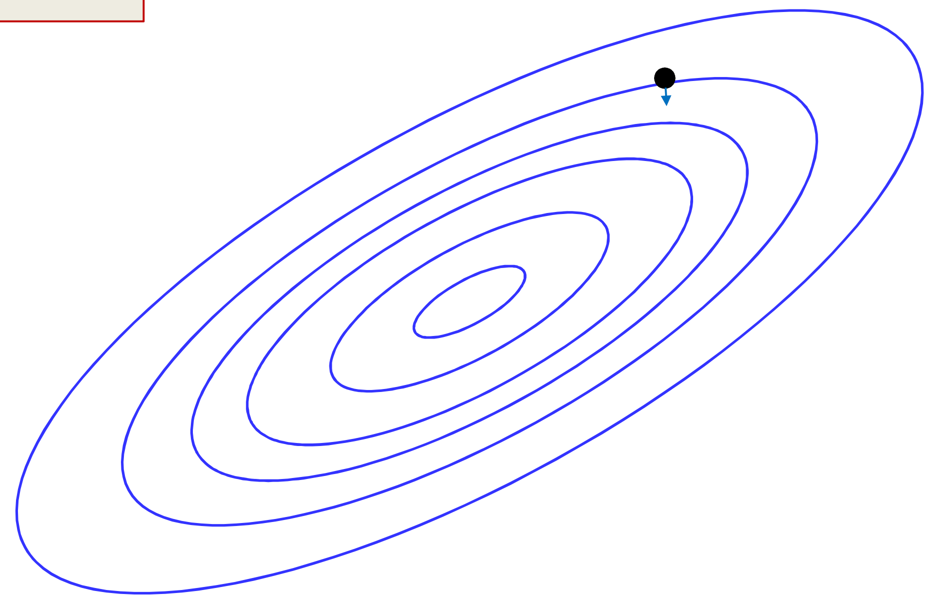
$$X_1 = X_2 = \cdots = X_T$$

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

The expected behavior of the gradient

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

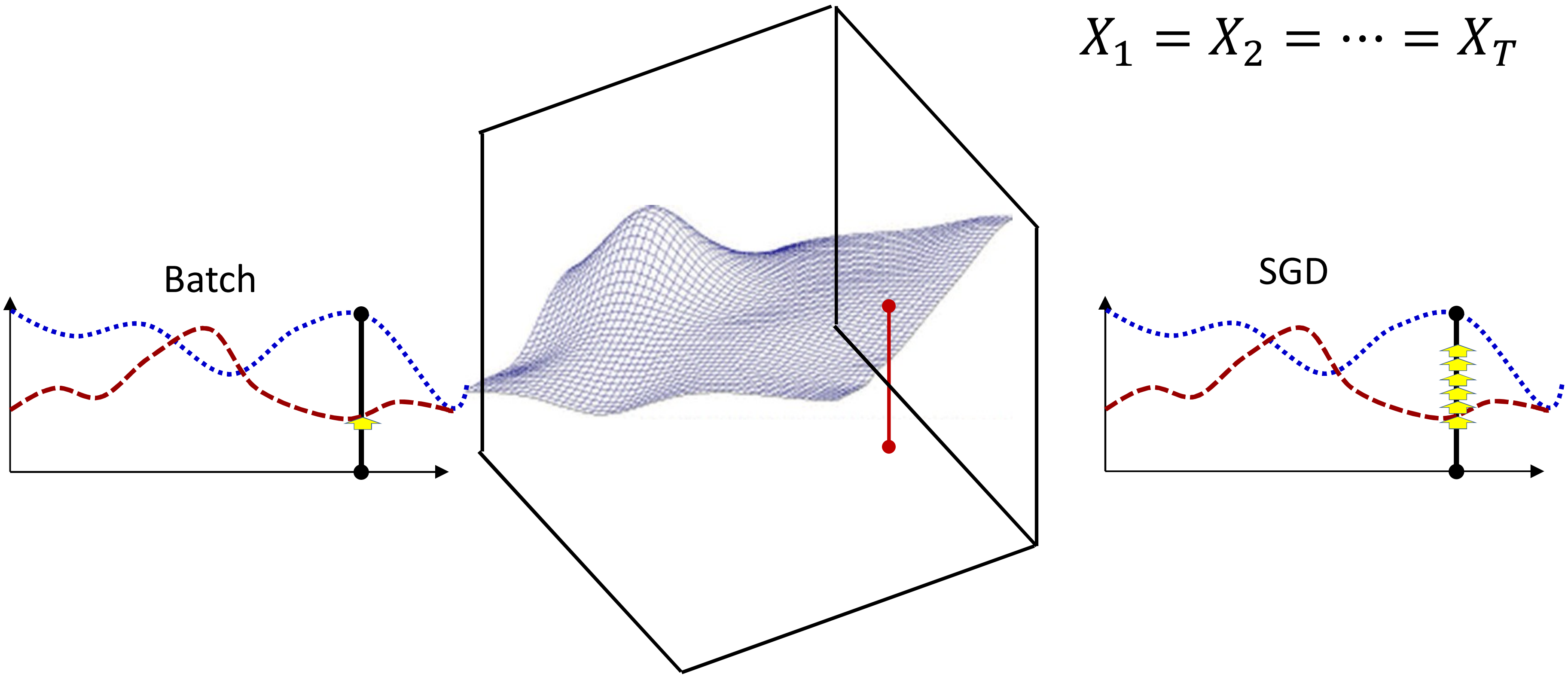




- The individual training instance contribute identical directions to the overall gradient
  - The final gradient points is simply the gradient for an individual instance

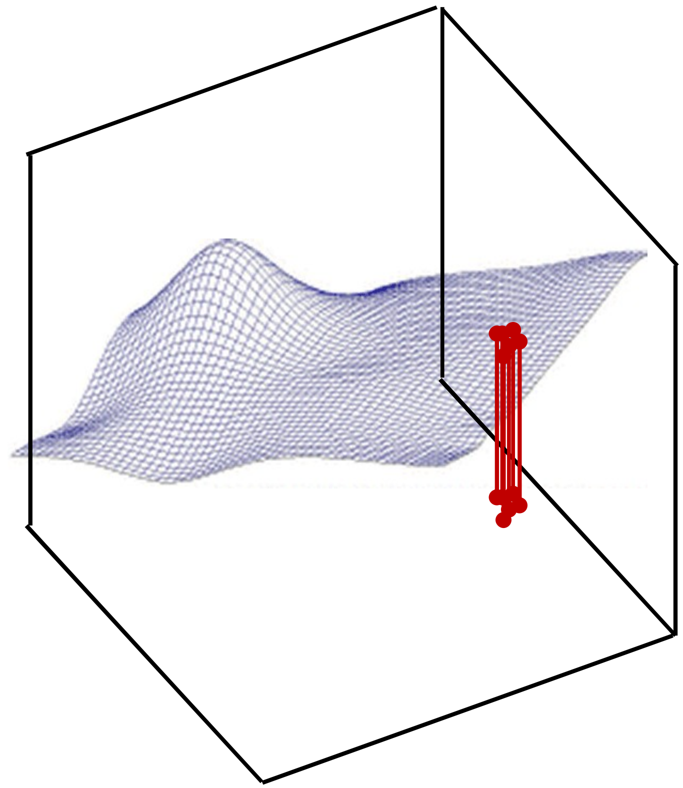
Batch vs SGD

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



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

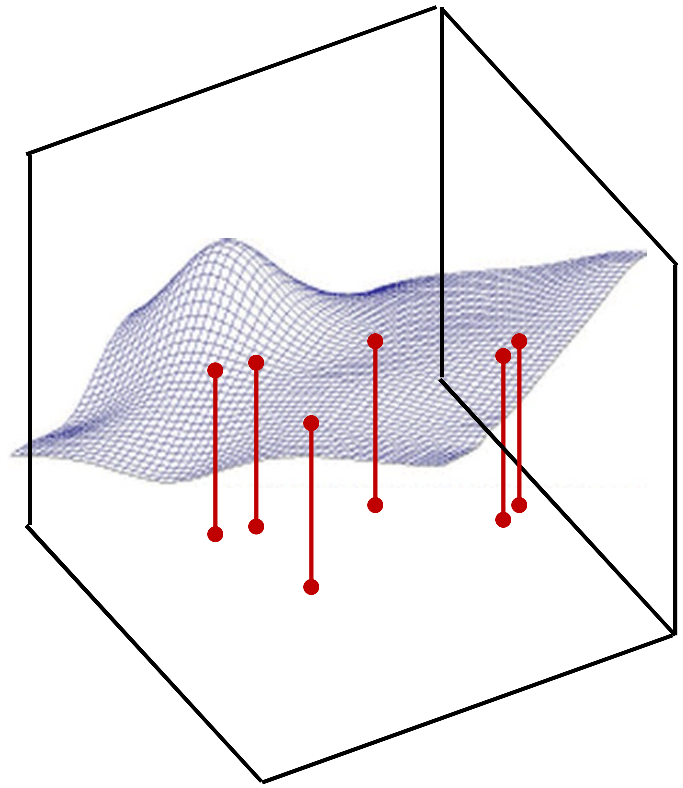
Clumpy data..



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

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

Clumpy data..



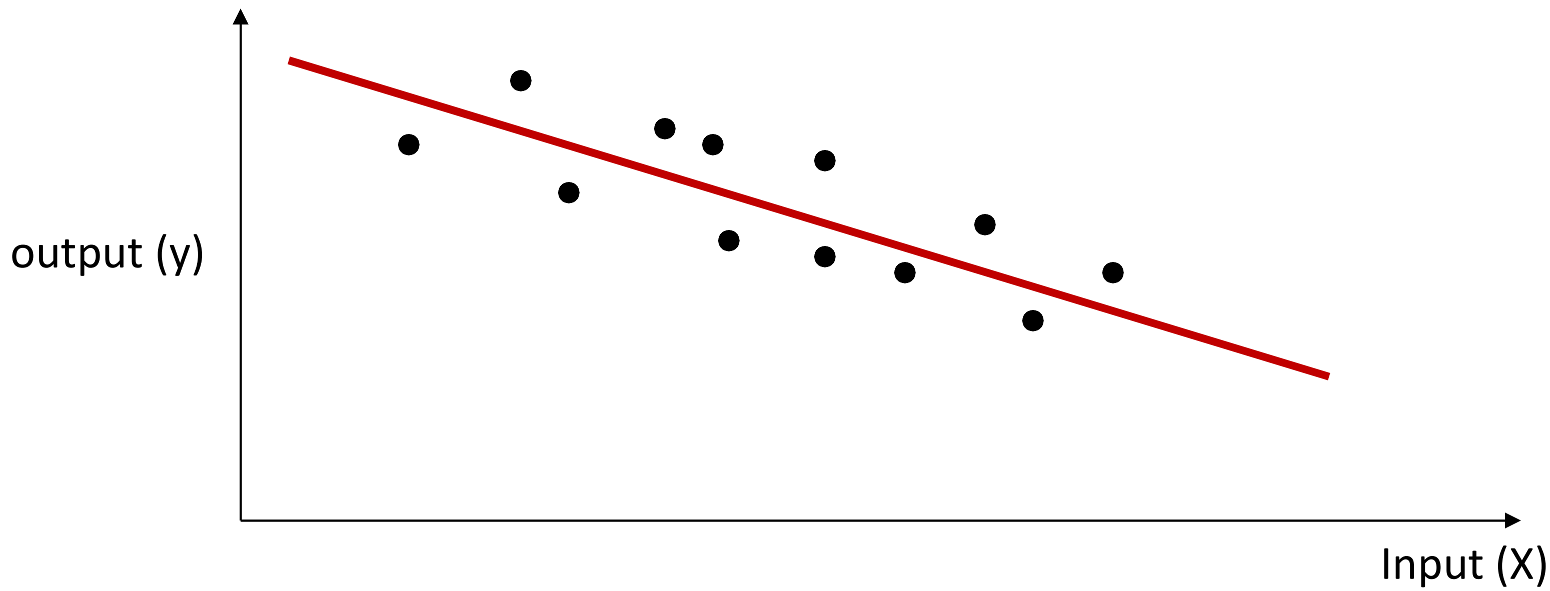
- As data get increasingly diverse, the benefits of incremental updates decrease, but do not entirely vanish

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),…, (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 all $t = 1{:}T$
    - $j = j + 1$
    - For every layer k:
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  - 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

$$\sum_k \eta_k = \infty$$

    - 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 error on the *entire* training data, although SGD itself updates after every training instance

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

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

  - 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,

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

  – 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

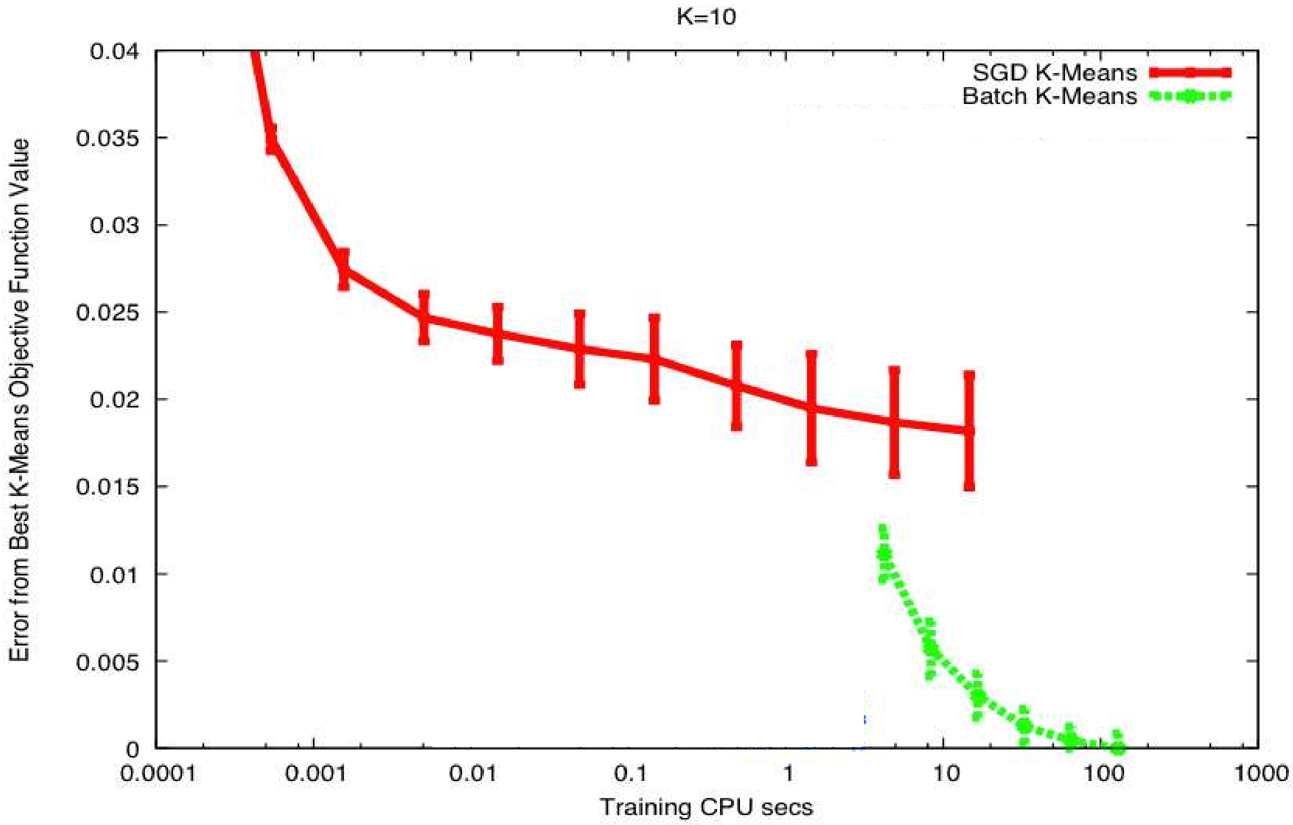
Polynomial Decay Averaging:

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

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

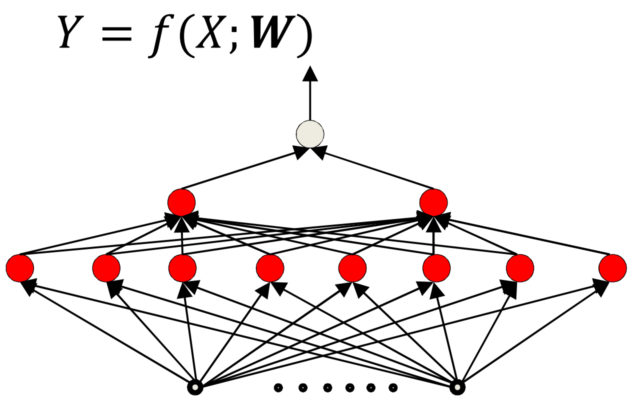
Achieves $\mathcal{O}\left(\frac{1}{T}\right)$ (strongly convex) and $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ (convex) convergence

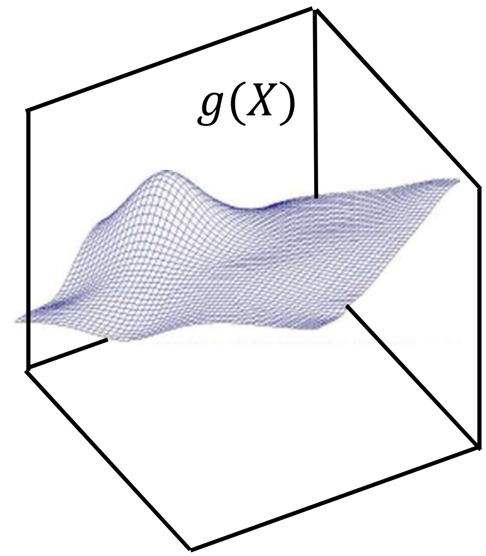
SGD example



- 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



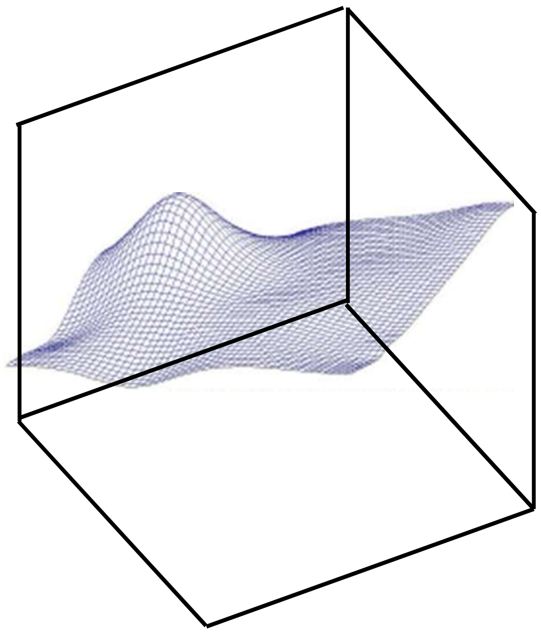


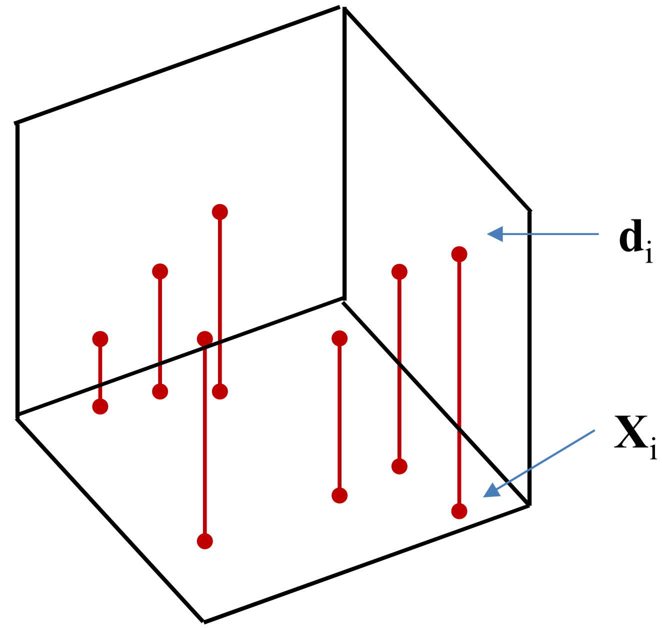
- To learn a network $f(X; \boldsymbol{W})$ to model a function $g(X)$ we minimize the *expected divergence*

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

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

Recall: The *Empirical* risk





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

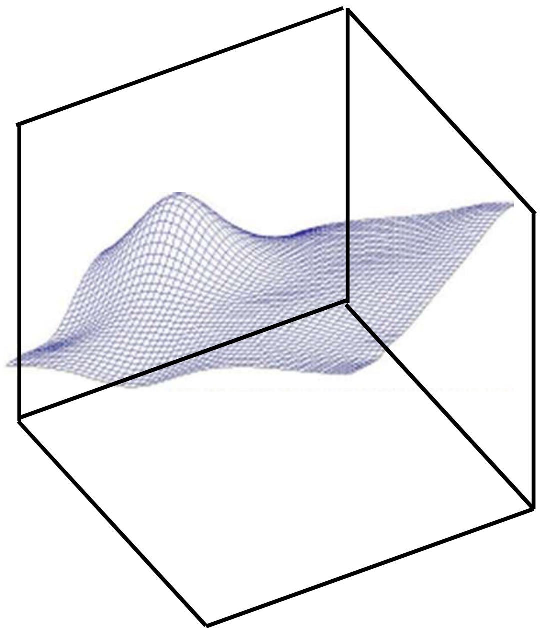
$$Loss(f(X;W), g(X)) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i;W), d_i)$$

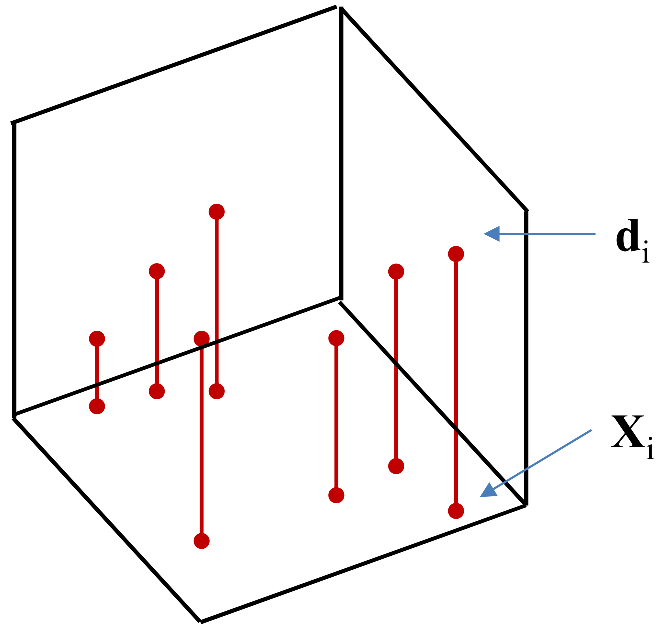
$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}}\, Loss(f(X;W), g(X))$$

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

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

Recall: The *Empirical* risk





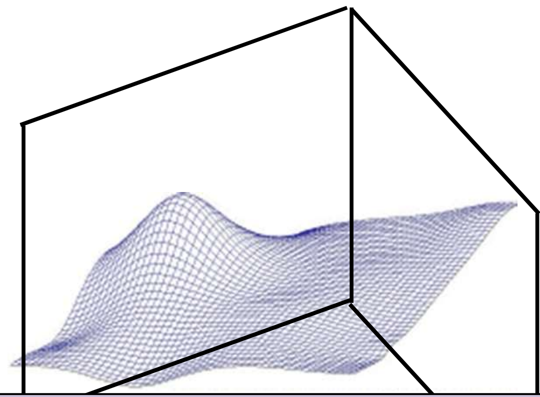
- In practice, we minimize the *empirical risk (or loss)*

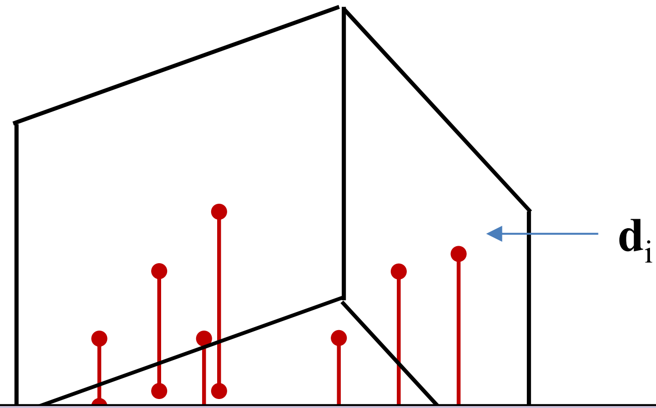
$$Loss\big(f(X;W), g(X)\big) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i;W), d_i)$$

The empirical risk is an *unbiased* estimate of the expected loss
Though there is no guarantee that minimizing it will minimize the expected loss

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

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 loss

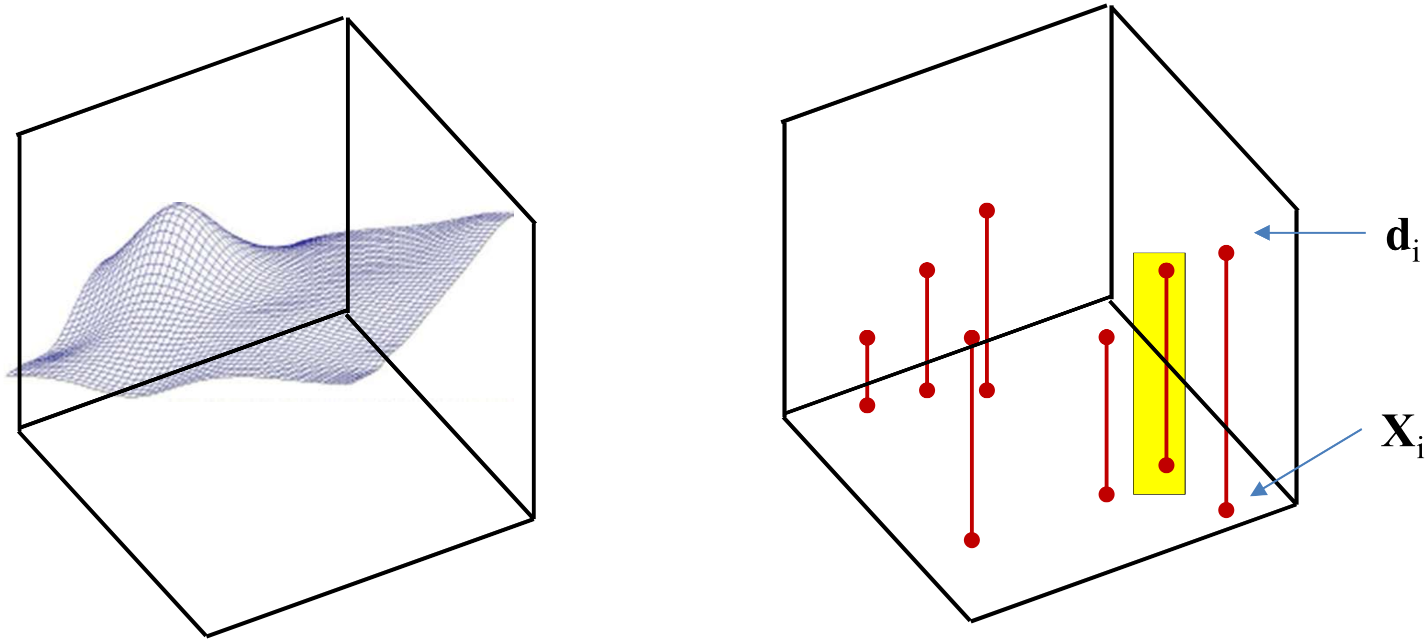
$$Loss\big(f(X;W), g(X)\big) = \frac{1}{N}\sum_{i=1}^{N} div(f(X_i;W), d_i)$$

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

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

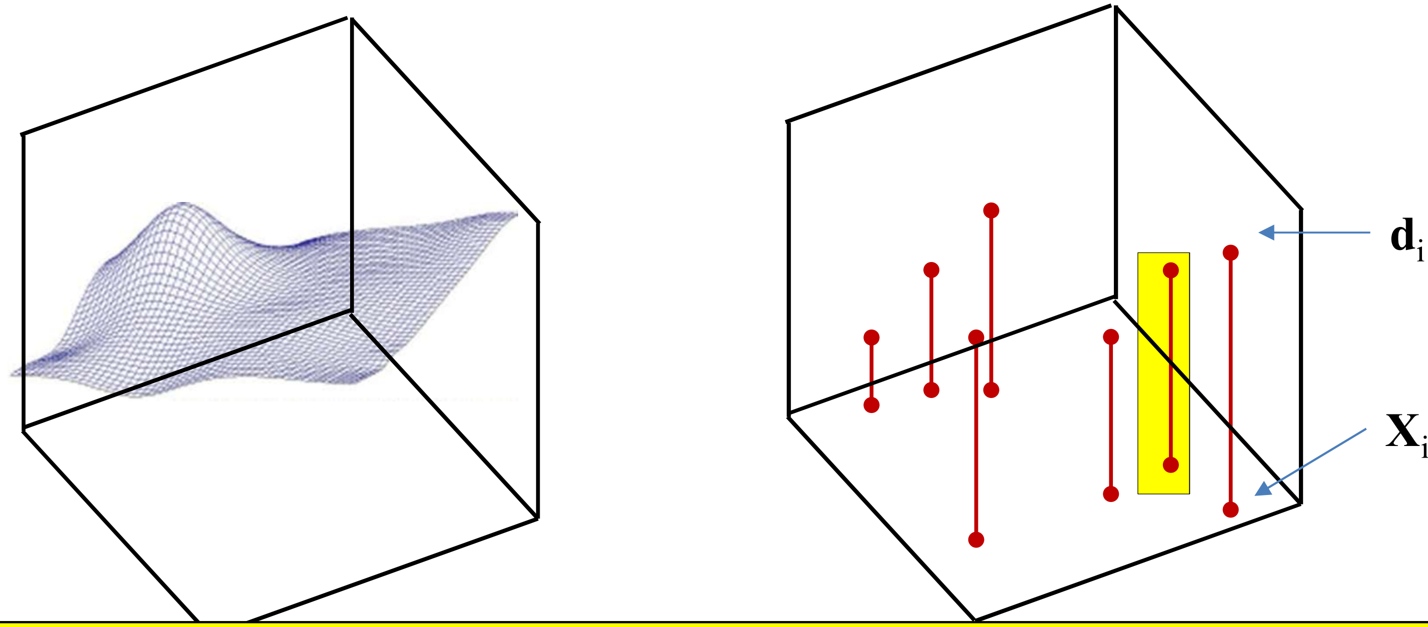
$$E\big[Loss\big(f(X;W), g(X)\big)\big] = E\big[div\big(f(X;W), g(X)\big)\big]$$

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 error 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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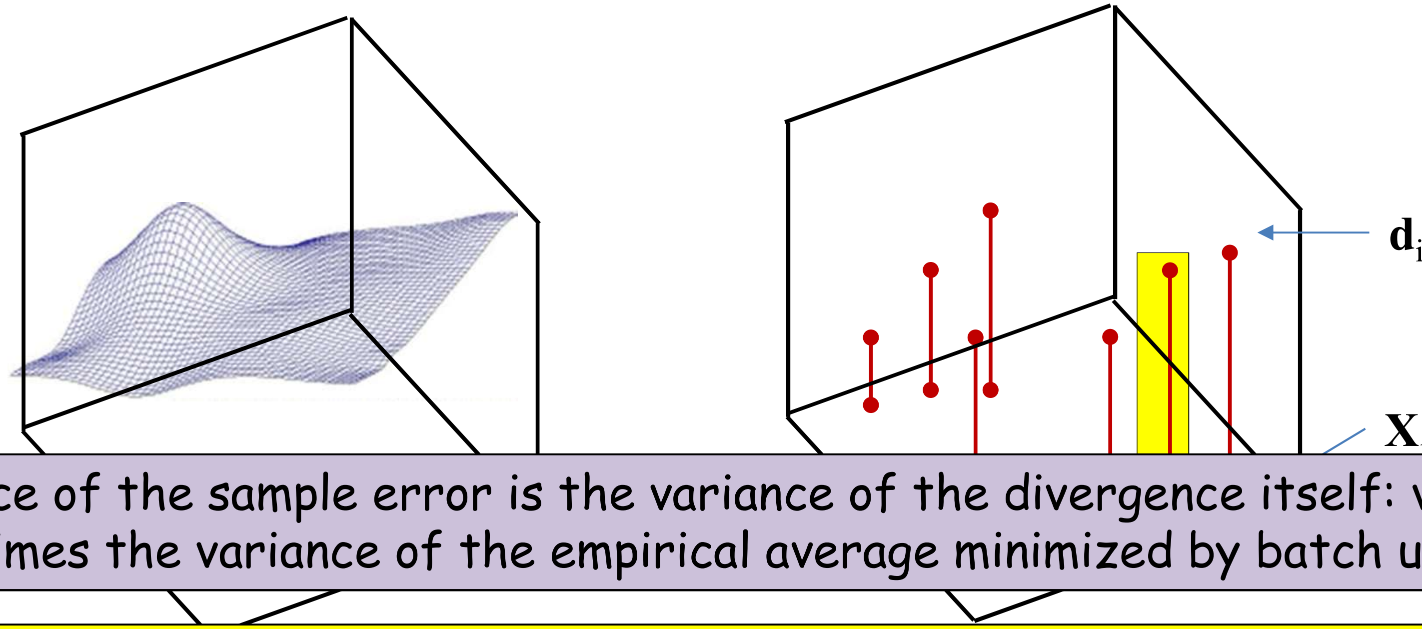
SGD

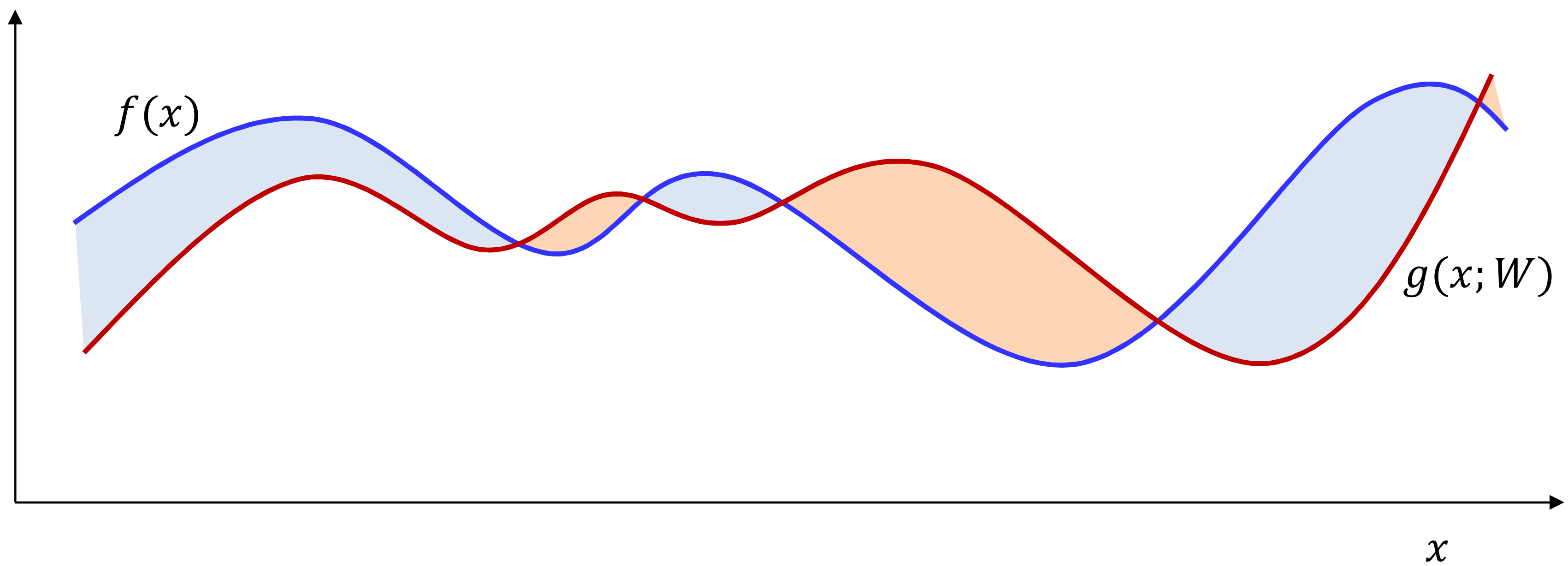


The variance of the sample error is the variance of the divergence itself: var(div)
This is N times the variance of the empirical average minimized by batch update

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

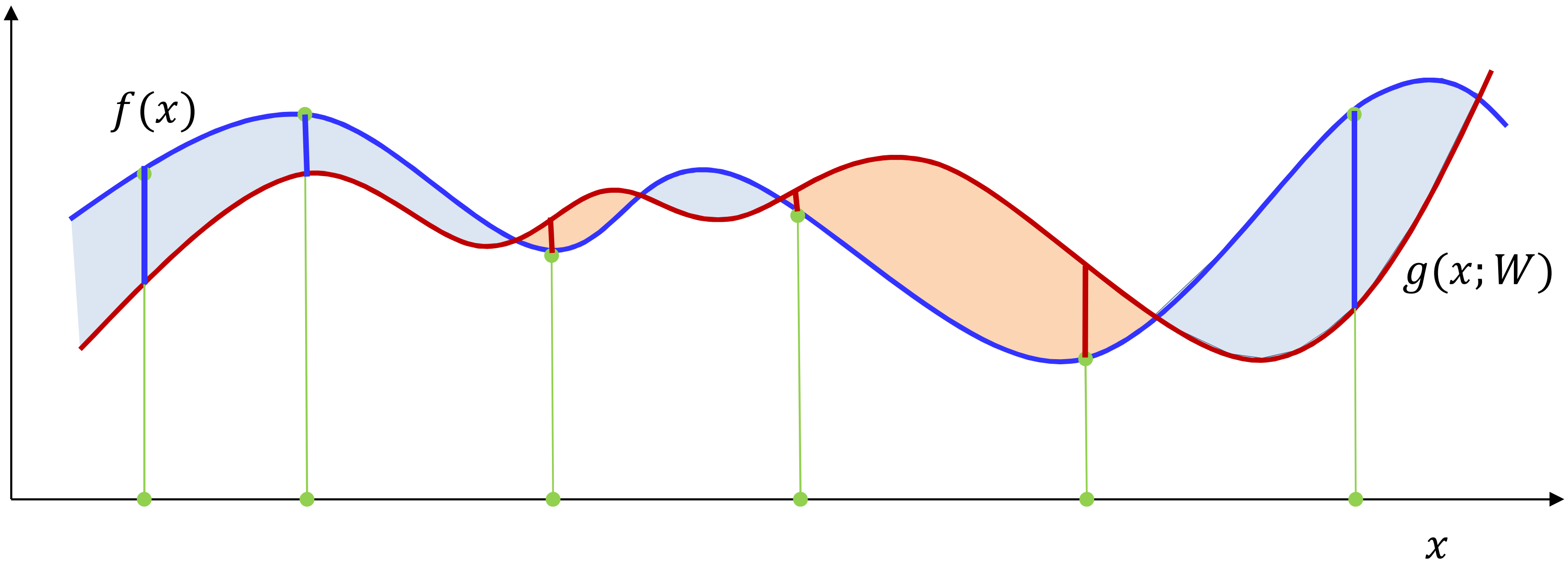
- At each iteration, **SGD** focuses on the divergence of a ***single*** sample $div(f(X_i; W), d_i)$
- The *expected value* of the *sample error* is ***still*** the *expected divergence* $E\left[div\left(f(X; W), g(X)\right)\right]$

Explaining the variance



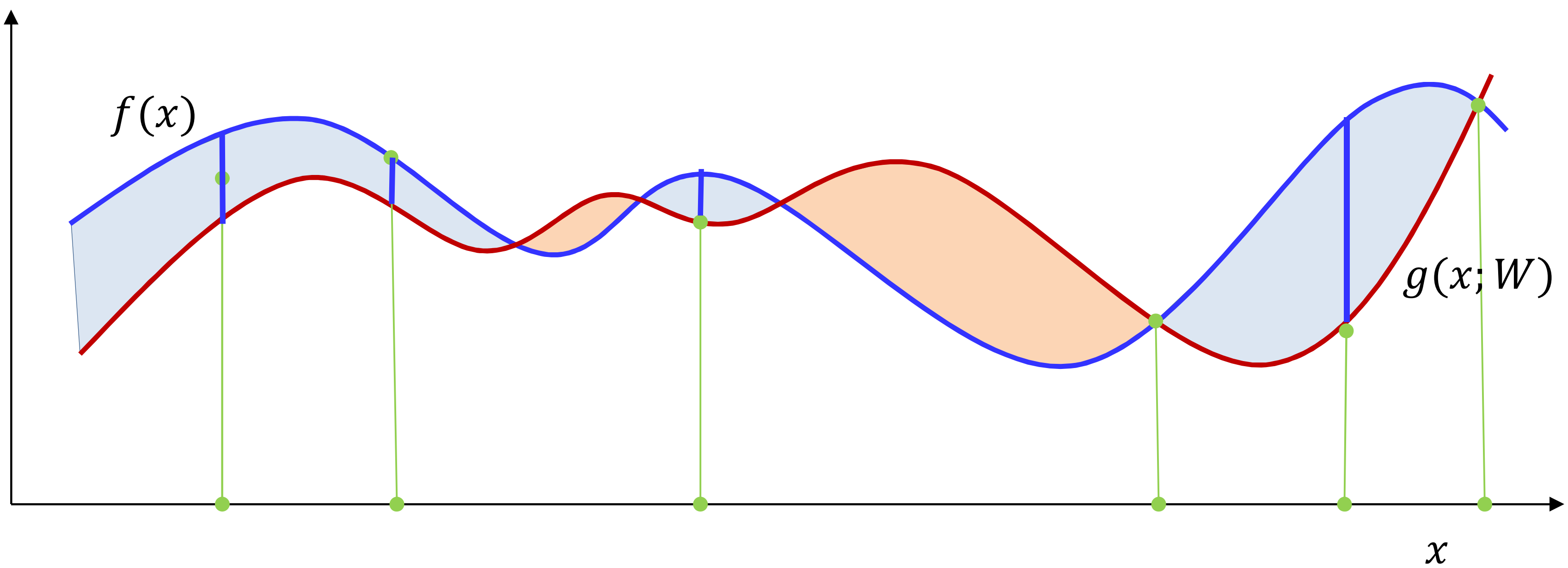
- The blue curve is the function being approximated
- The red curve is the approximation by the model at a given W
- The heights of the shaded regions represent the point-by-point error
  – The divergence is a function of the error
  – We want to find the W that minimizes the average divergence

Explaining the variance



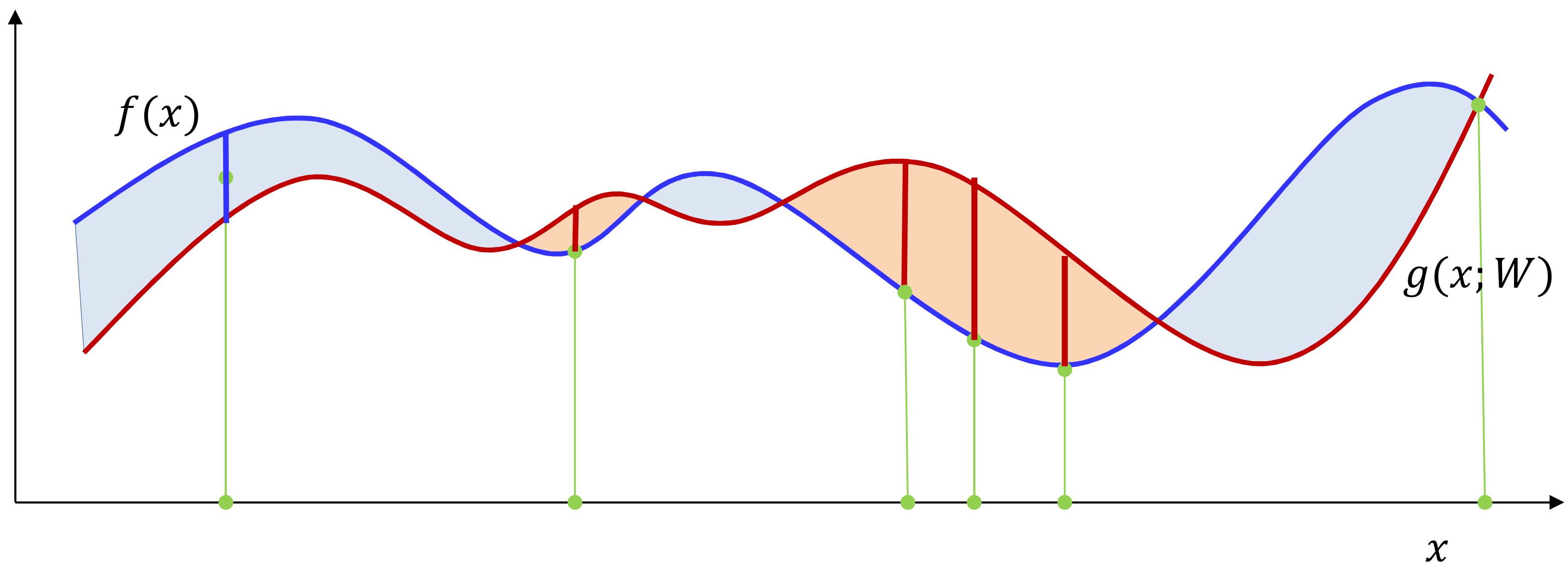
- Sample estimate approximates the shaded area with the average length of the lines

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
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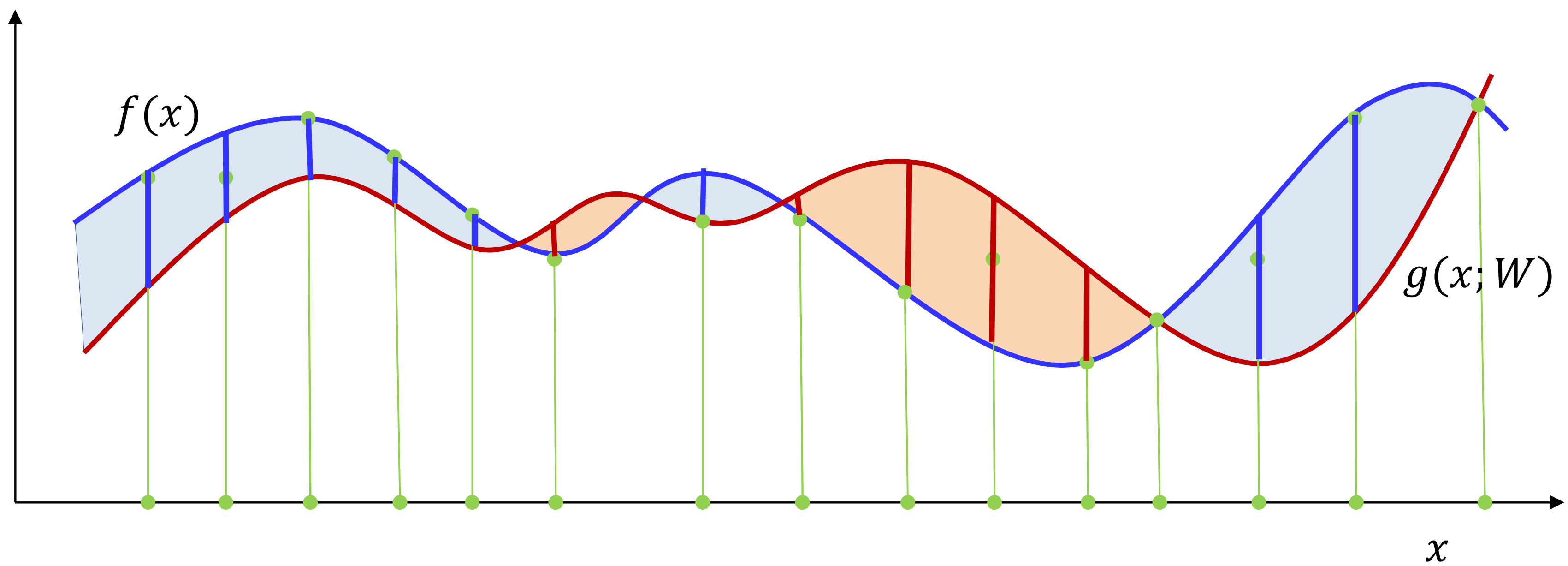
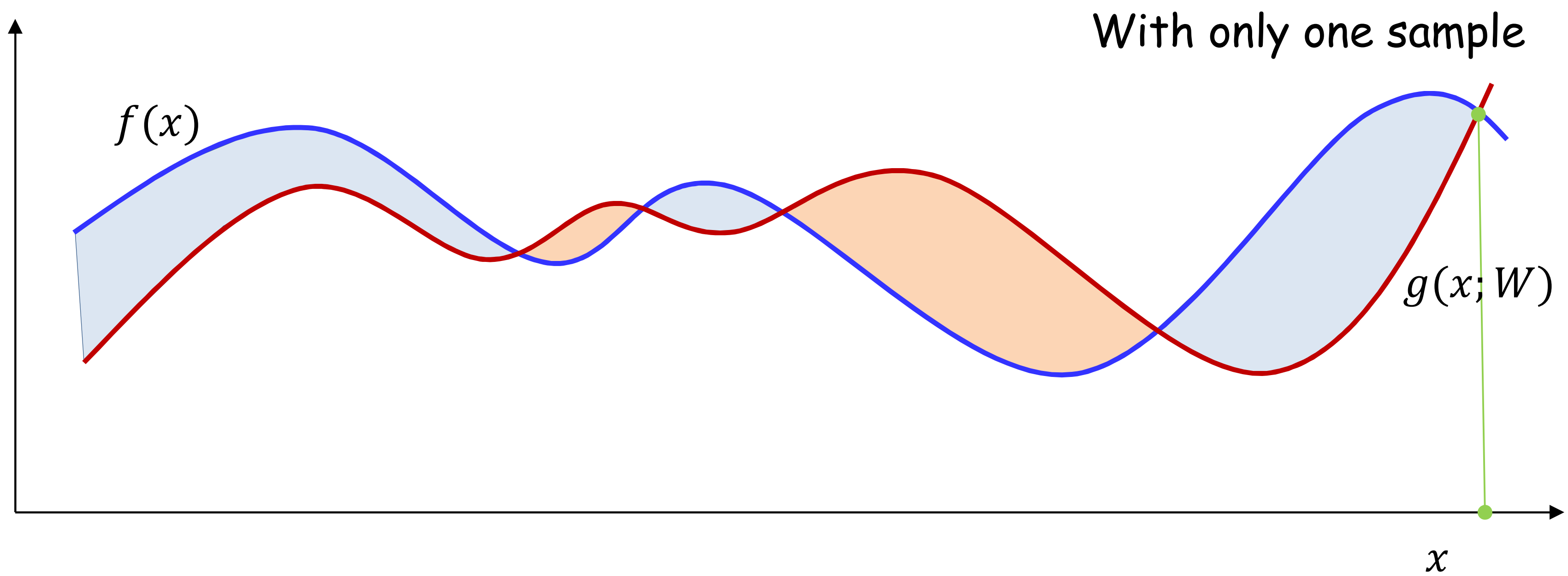
Explaining the variance



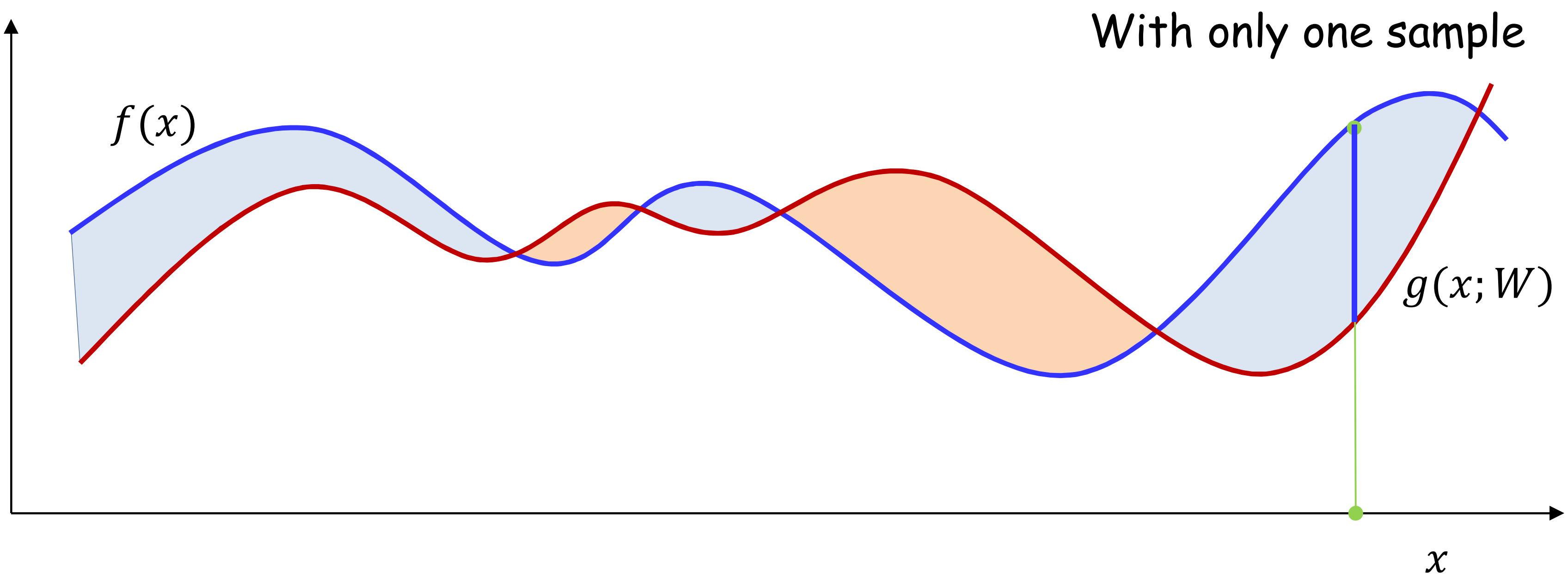
- Having more samples makes the estimate more robust to changes in the position of samples
  - The variance of the estimate is smaller

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



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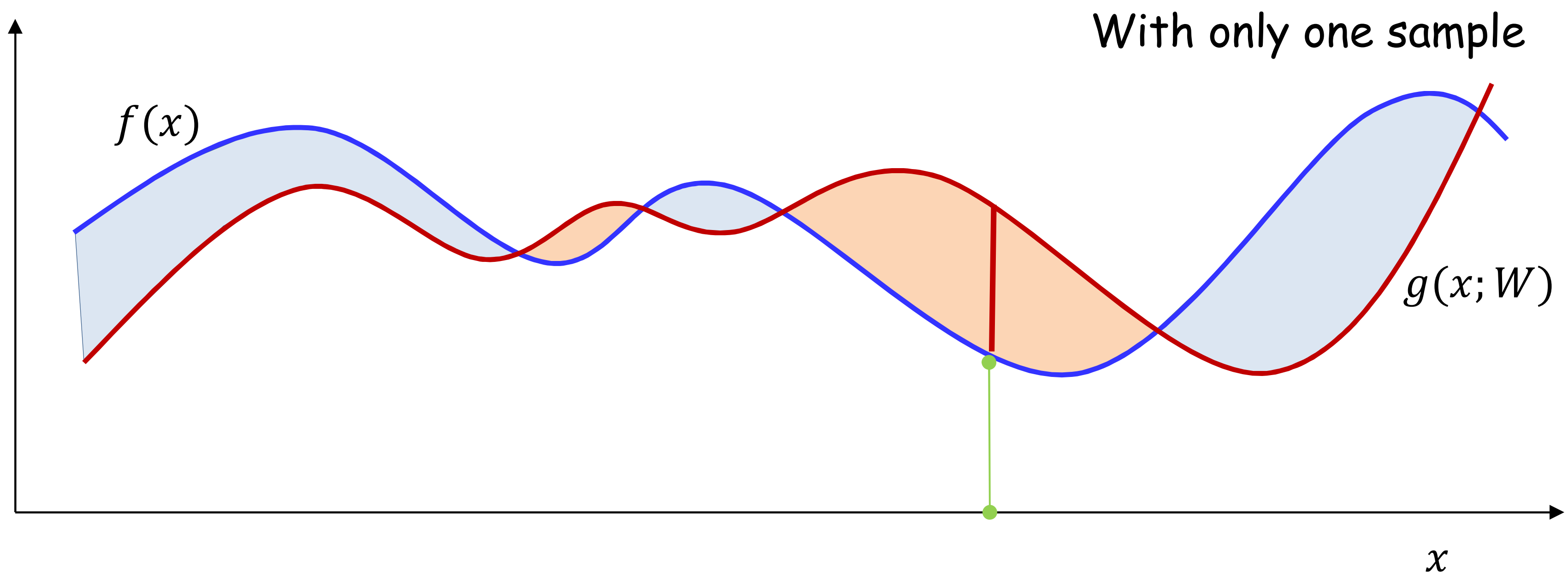
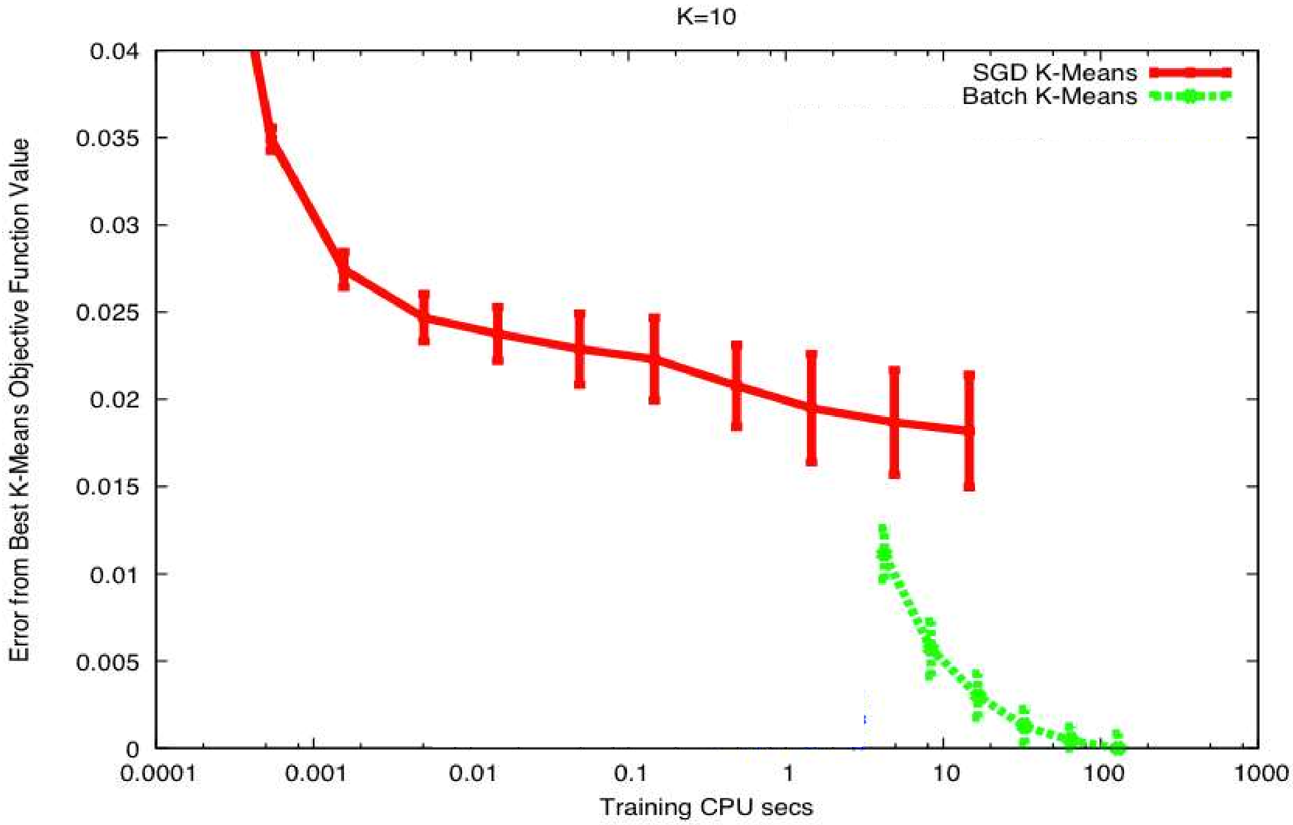
Explaining the variance



- 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



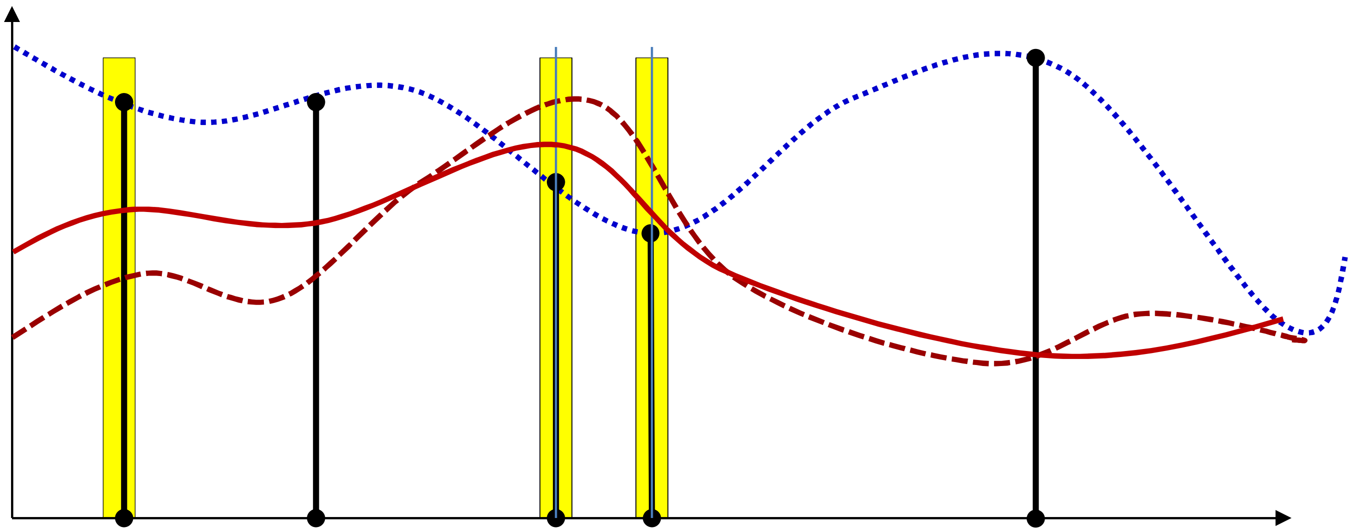
- A simpler problem: K-means
- Note: SGD converges slower
- Also has large variation between runs

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

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 $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
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        - » $\Delta W_k = \Delta W_k + \frac{1}{b} \nabla_{W_k} Div(Y_t, d_t)^T$
    - Update
      - For every layer k:

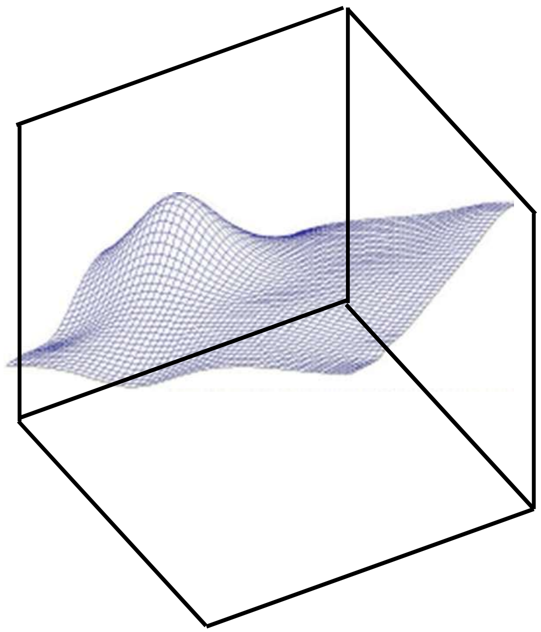
$$W_k = W_k - \eta_j \Delta W_k$$

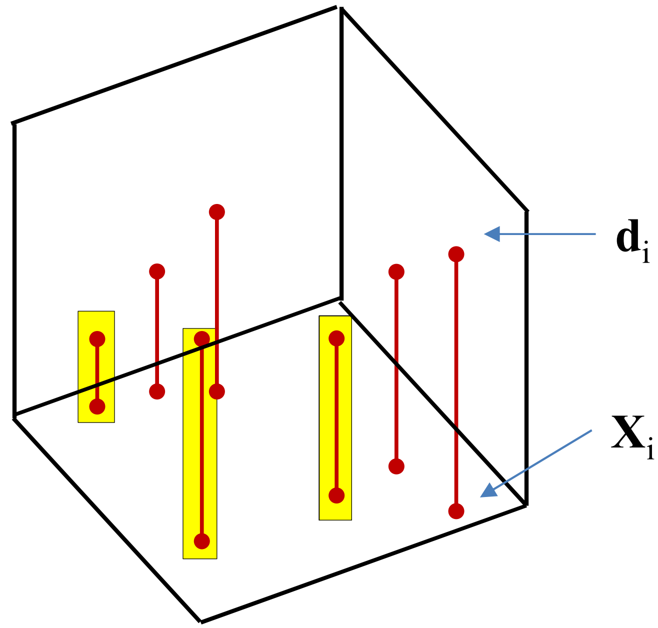
- Until Err has converged

Mini-batch size

Shrinking step size

Mini Batches





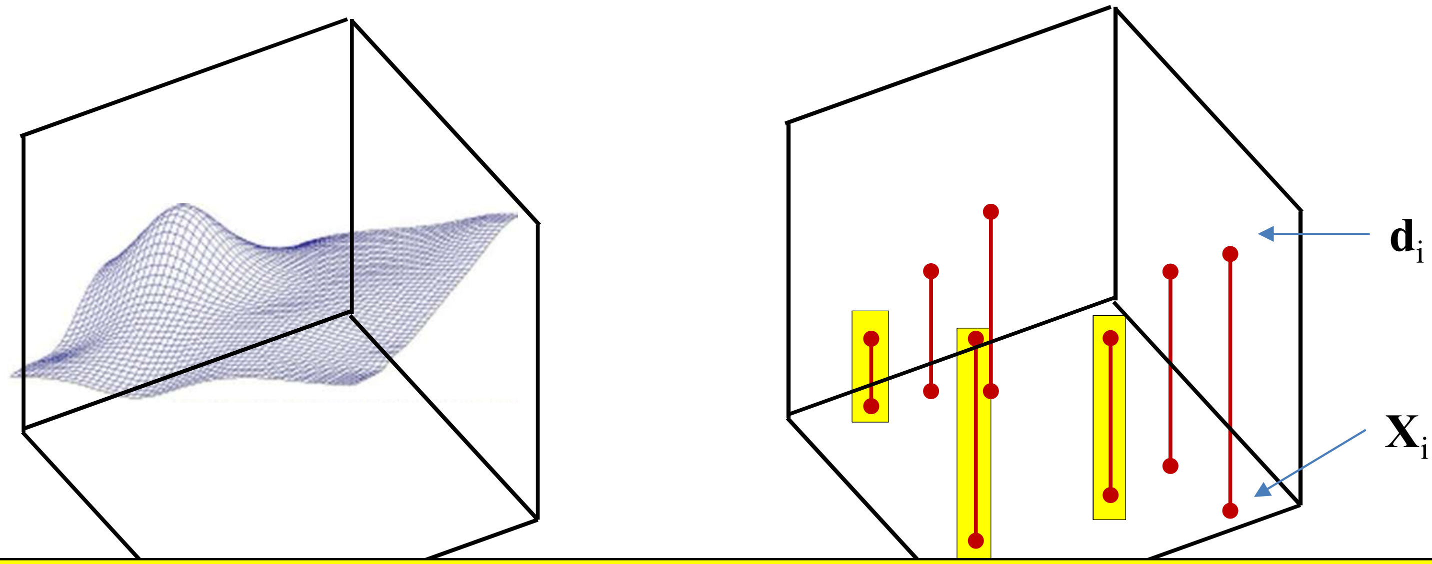
- Mini-batch updates compute and minimize a *batch loss*

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

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

$$E[BatchLoss(f(X;W), g(X))] = E[div(f(X;W), g(X))]$$

Mini Batches



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

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

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

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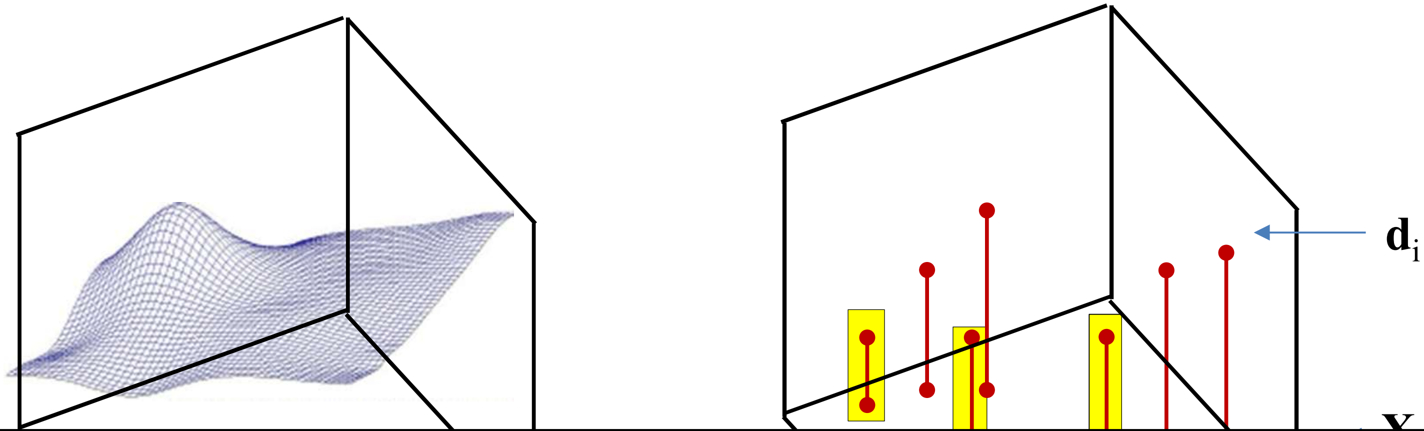
Mini Batches



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

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

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

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

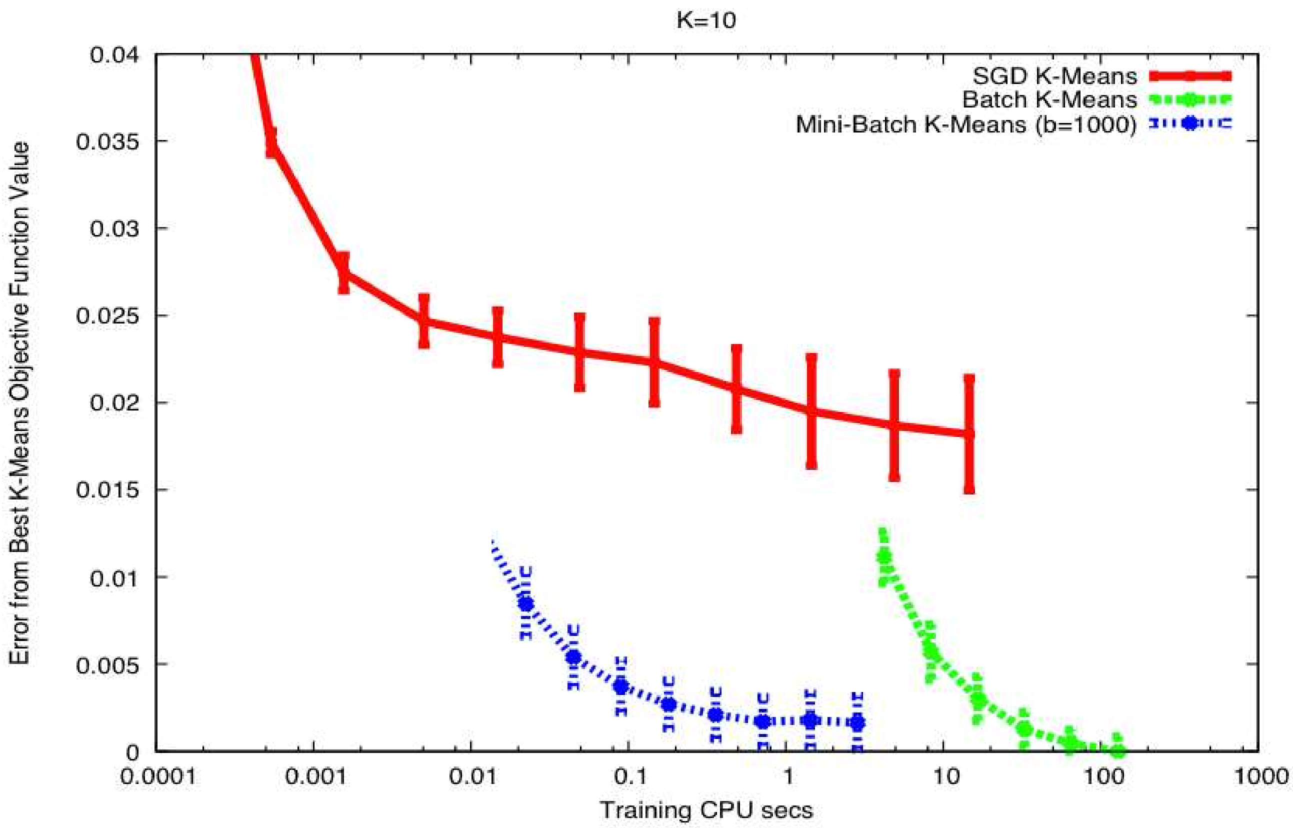
- The *expected value* of the *batch loss* is also the *expected divergence*

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

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

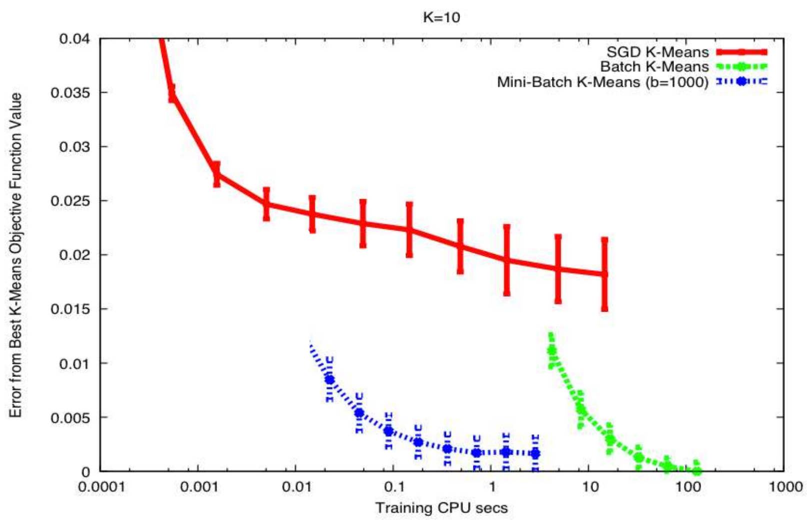
SGD example



- 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

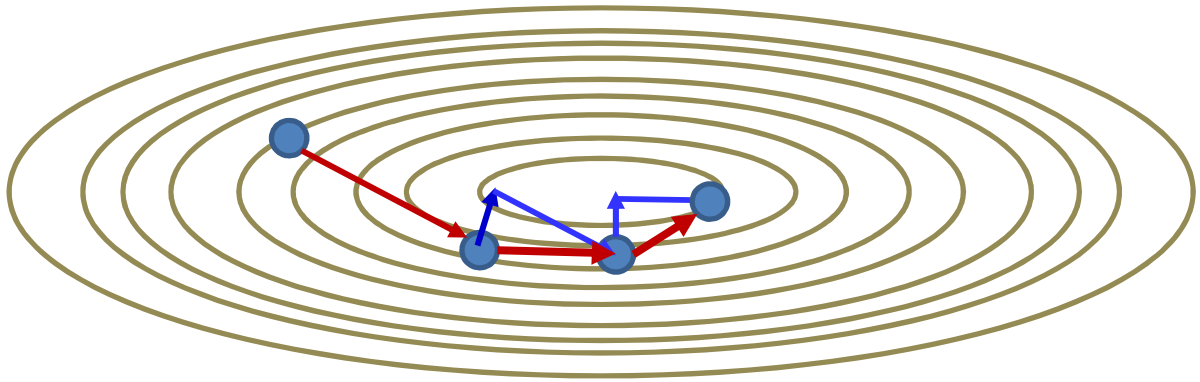
Training and minibatches

- 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

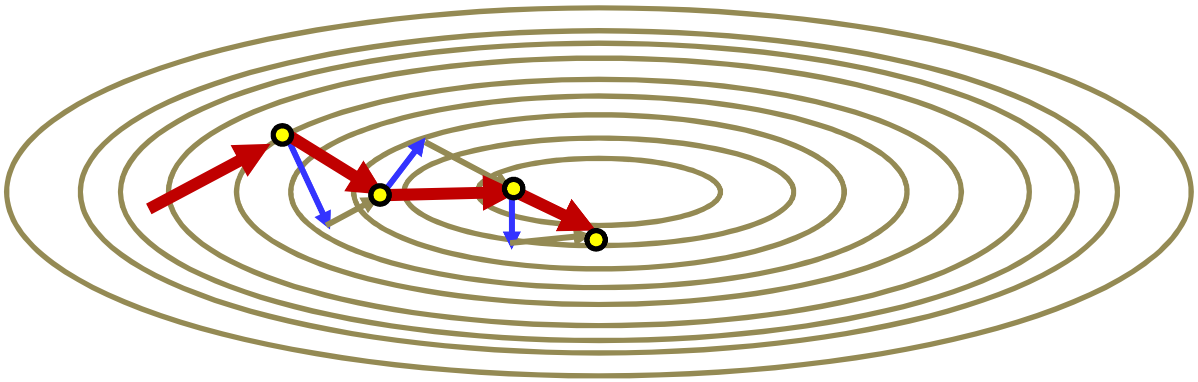


- The momentum method

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

- Updates using a running average of the gradient

Momentum and incremental updates



- 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

Incremental Update: Mini-batch update

- Given (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$, $\Delta W_k = 0$
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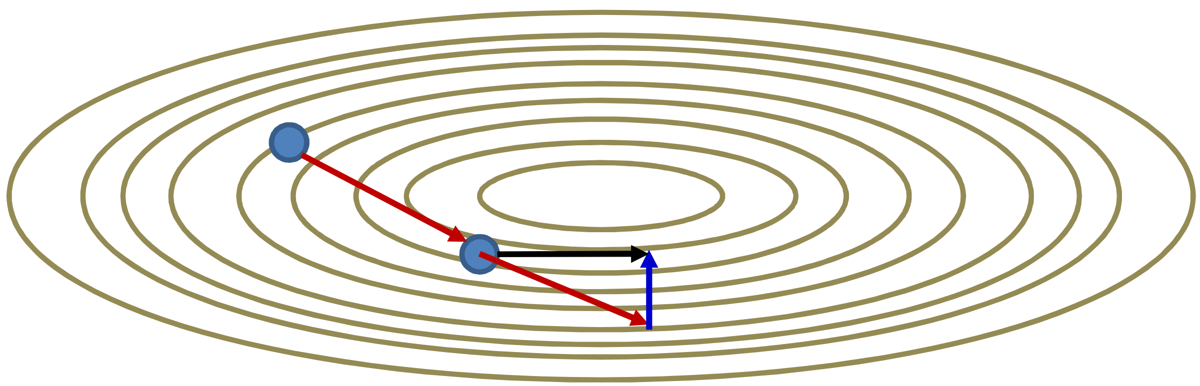
      - For every layer k:
        - » Compute $\nabla_{W_k} Div(Y_t, d_t)$
        - » $\nabla_{W_k} Loss \mathrel{+}= \frac{1}{b} \nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
    - Update
      - For every layer k:

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

$$W_k = W_k + \Delta W_k$$

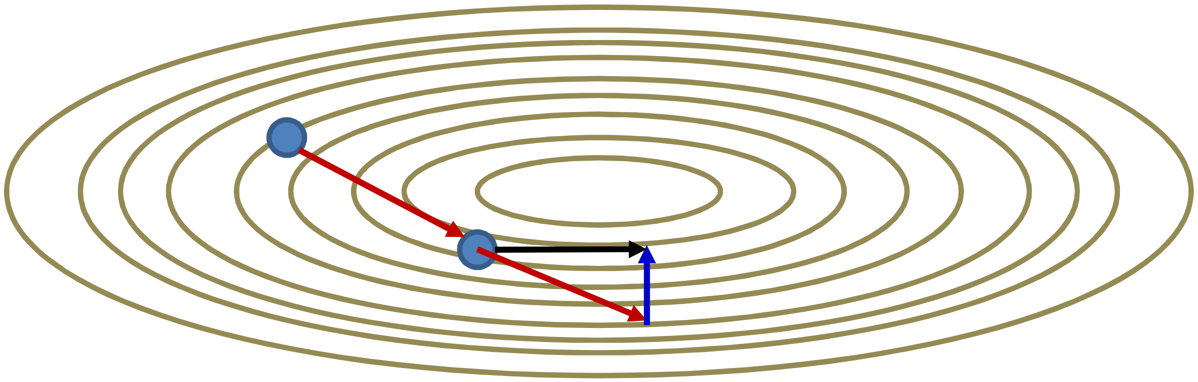
- Until $Loss$ has converged

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



- Nestorov's method

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

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

Incremental Update: Mini-batch update

- Given $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$, $\Delta W_k = 0$
- 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:
      - $W_k = W_k + \beta \Delta W_k$
      - $\nabla_{W_k} Loss = 0$
    - 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:

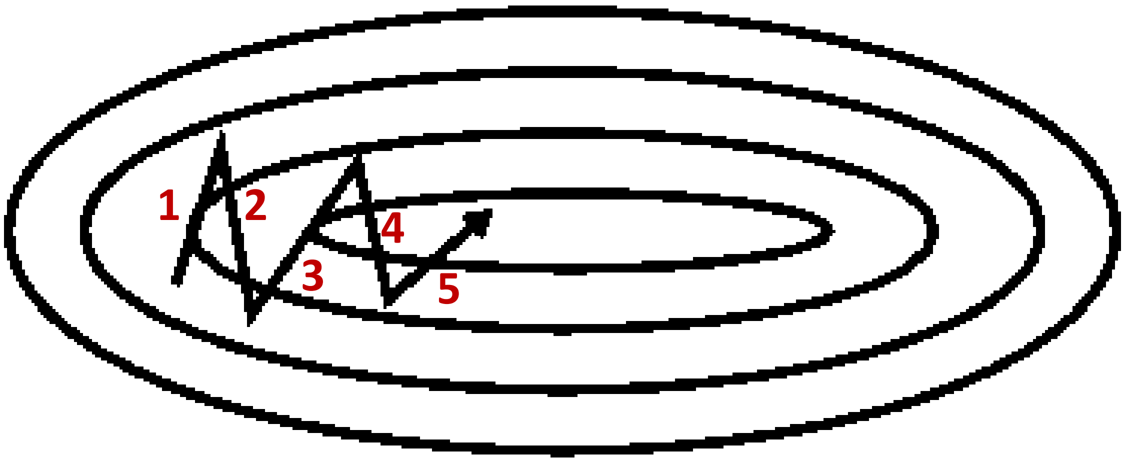
$$W_k = W_k - \eta_j \nabla_{W_k} Loss^T$$
$$\Delta W_k = \beta \Delta W_k - \eta_j \nabla_{W_k} Loss^T$$

- Until $Loss$ has converged

More recent methods

- Several newer methods have been proposed that follow the general pattern of enhancing long-term trends to smooth out the variations of the mini-batch gradient
  - RMS Prop
  - Adagrad
  - AdaDelta
  - ADAM: very popular in practice
  - …
- All roughly equivalent in performance

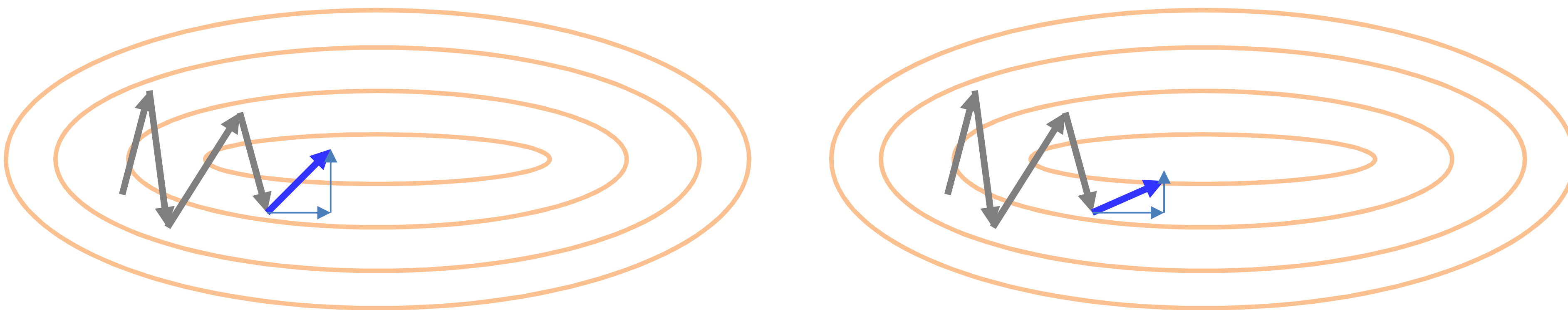
Smoothing the trajectory



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

- Simple gradient and acceleration methods still demonstrate oscillatory behavior in some directions
- 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
- Improvement: Dampen step size in directions with high motion
  - ***Second order term***

Variance-normalized step



- In recent past
  - Total movement in *Y* component of updates is high
  - Movement in *X* components is lower
- Current update, modify usual gradient-based update:
  - Scale *down* Y component
  - Scale *up* X component
  - *According to their variation (and not just their average)*
- A variety of algorithms have been proposed on this premise
  - We will see a popular example

RMS Prop

- Notation:
  - Updates are ***by parameter***
  - Sum derivative of divergence w.r.t any individual parameter w is shown as $\partial_w D$
  - 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

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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 $\boldsymbol{Y}(\boldsymbol{X}_{t+b})$
        - » Compute gradient $\frac{d\boldsymbol{Div}(\boldsymbol{Y}(\boldsymbol{X}_{t+b}),\boldsymbol{d}_{t+b})}{d\boldsymbol{w}}$
        - » Compute$(\partial_w D)_k$ $+= \frac{1}{B}\frac{d\boldsymbol{Div}(\boldsymbol{Y}(\boldsymbol{X}_{t+b}),\boldsymbol{d}_{t+b})}{d\boldsymbol{w}}$
    - update:

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

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

    - $k = k + 1$
- Until $E(\boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}, \ldots, \boldsymbol{W}^{(K)})$ has converged

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 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 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

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

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

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

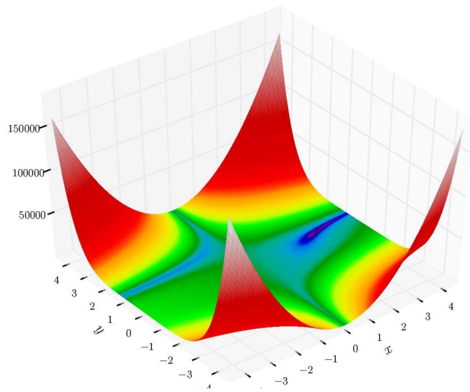
$$w_{k+1} = w_k - \frac{\eta}{\sqrt{\hat{v}_k + \epsilon}}\hat{m}_k$$

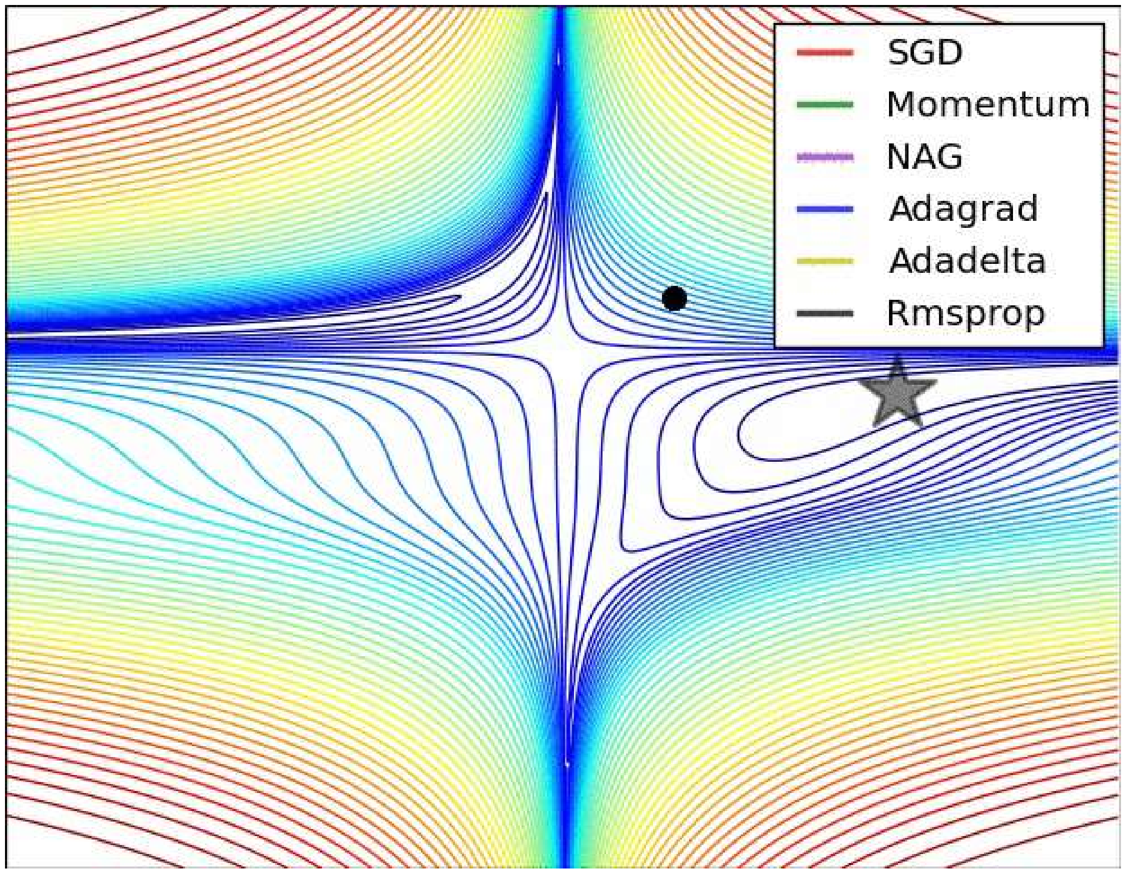
Ensures that the δ and γ terms do not dominate in early iterations

Other variants of the same theme

- Many:
  - Adagrad
  - AdaDelta
  - ADAM
  - 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: $\eta = 0.001, \delta = 0.9, \gamma = 0.999$

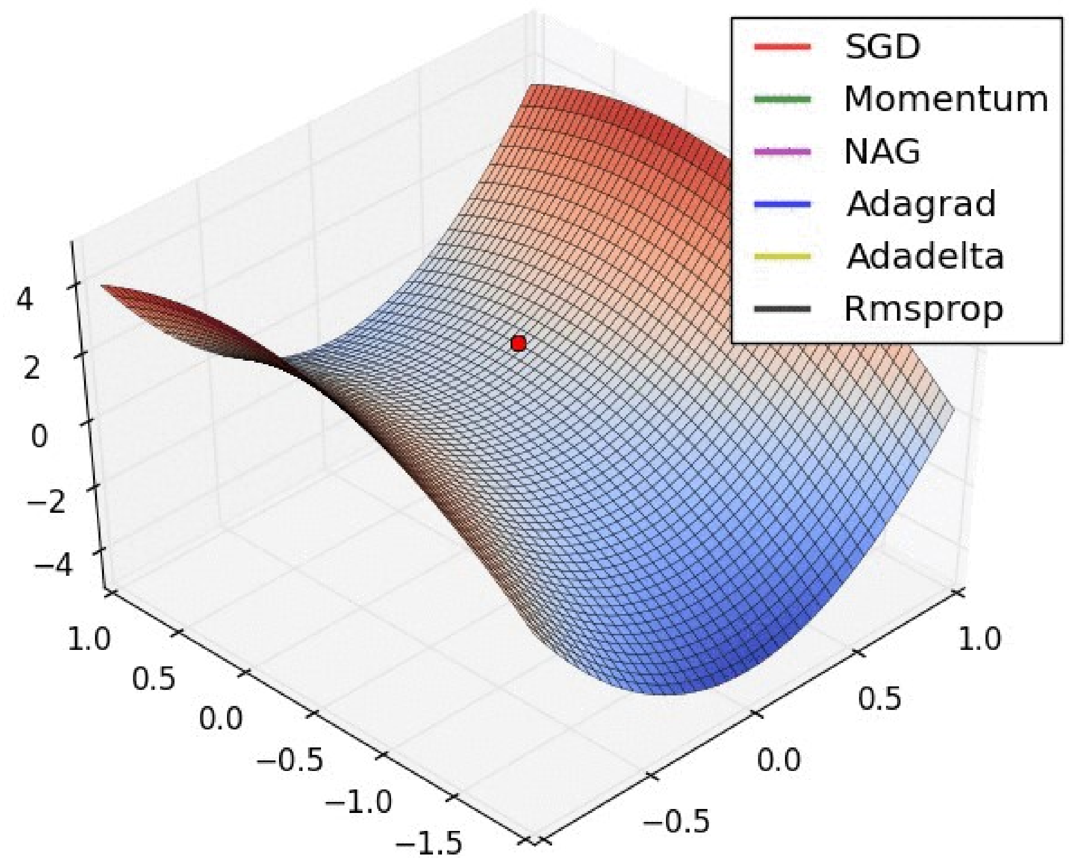
Visualizing the optimizers: Beale's Function





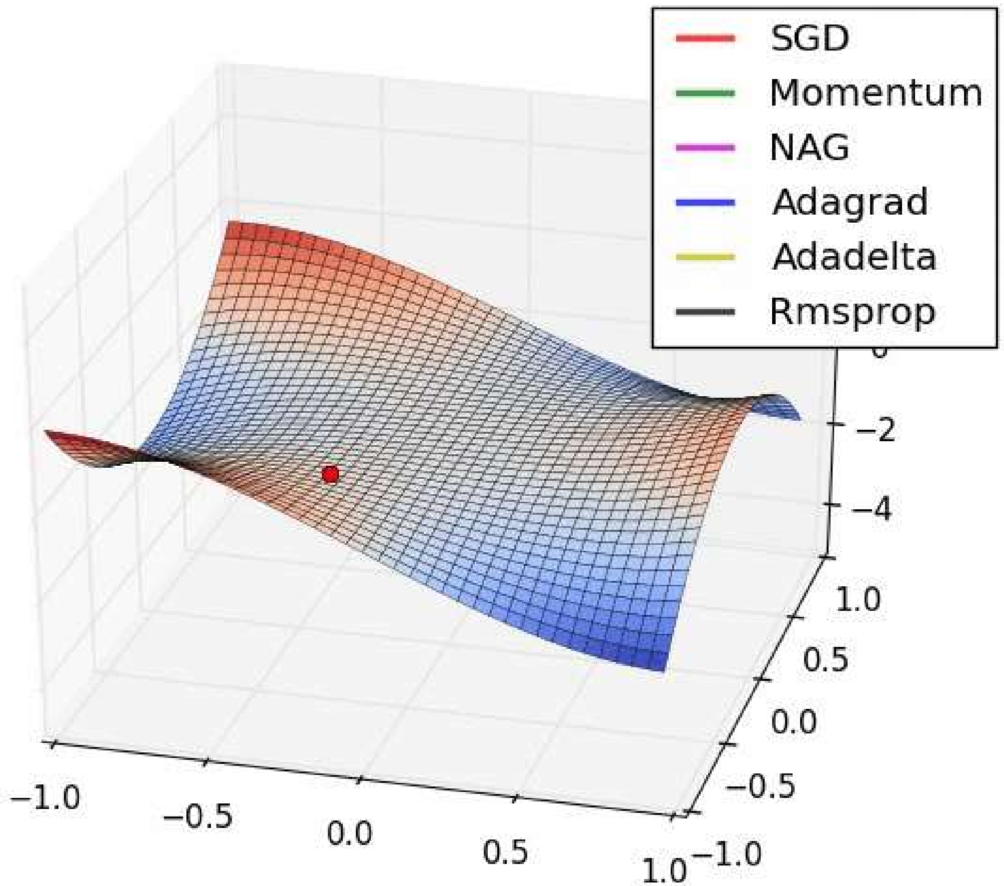
- http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

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

Moving on: Topics for the day

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

Tricks of the trade..

- To make the network converge better
  - The Divergence
  - Dropout
  - Batch normalization
  - Other tricks
    - Gradient clipping
    - Data augmentation
    - Other hacks..

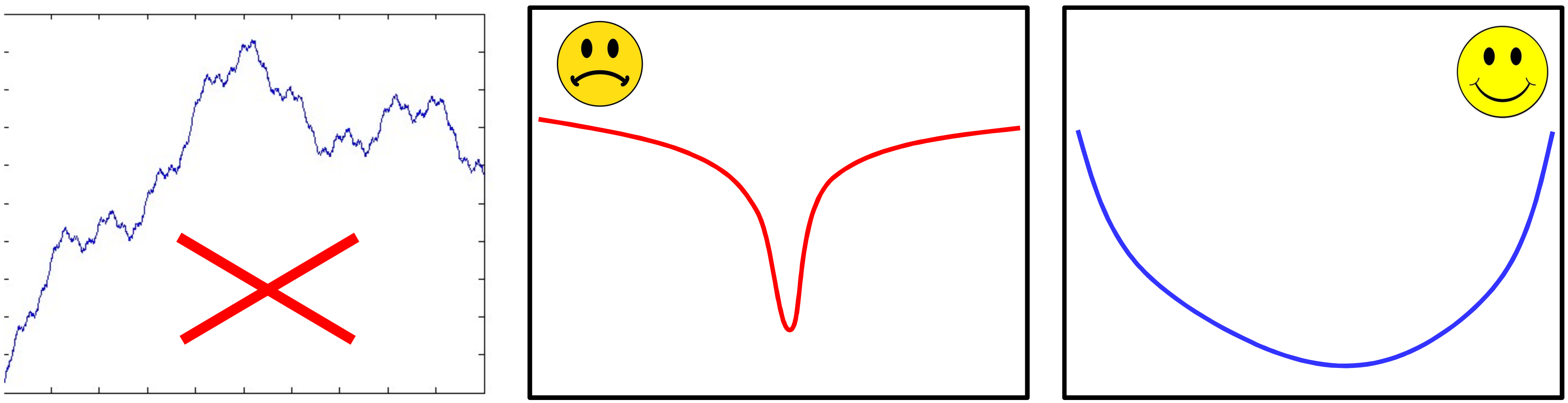
Training Neural Nets by Gradient Descent: The Divergence

Total training loss:

$$Loss = \frac{1}{T}\sum_{t} Div(Y_t, d_t; \mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_K)$$

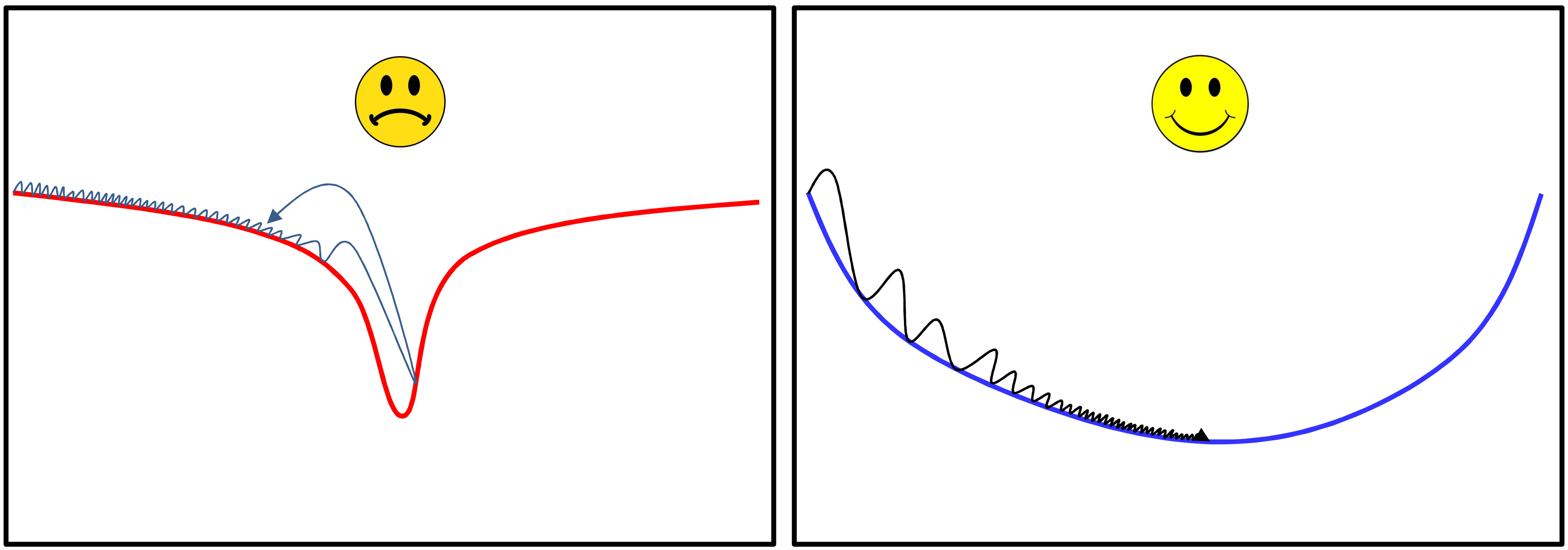
- The convergence of the gradient descent depends on the divergence
  - Ideally, must have a shape that results in a significant gradient in the right direction outside the optimum
    - To “guide” the algorithm to the right solution

Desiderata for a good divergence



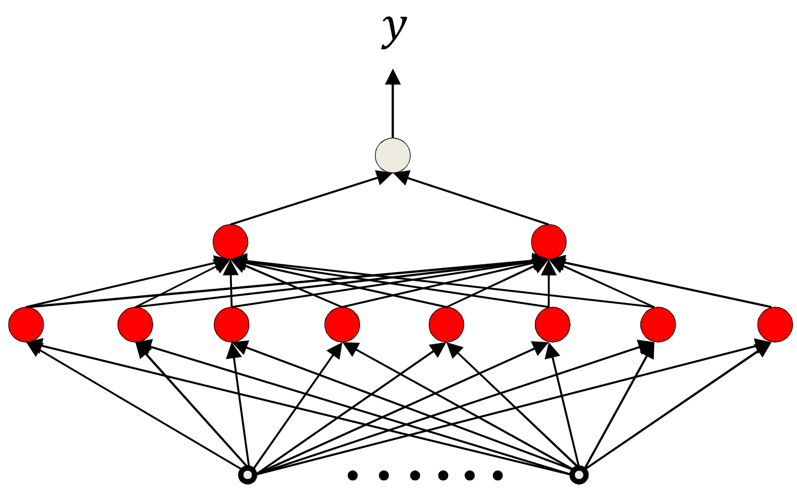
- Must be smooth and not have many poor local optima
- Low slopes far from the optimum == bad
  - Initial estimates far from the optimum will take forever to converge
- High slopes near the optimum == bad
  - Steep gradients

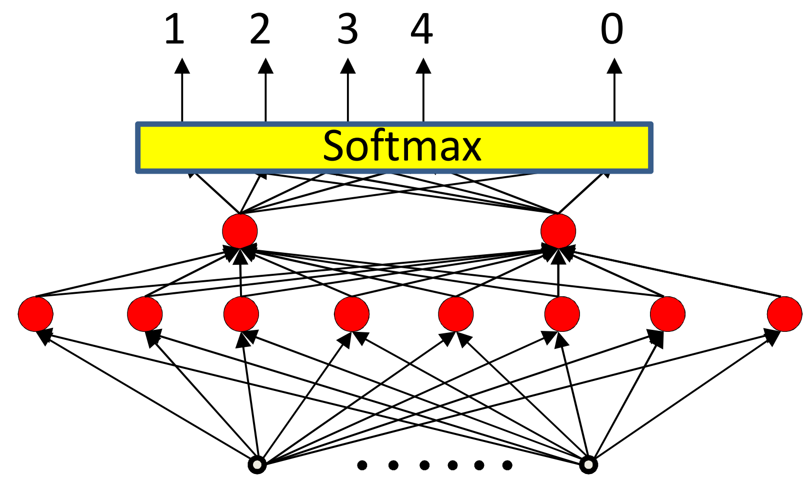
Desiderata for a good divergence



- Functions that are shallow far from the optimum will result in very small steps during optimization
  - Slow convergence of gradient descent
- Functions that are steep near the optimum will result in large steps and overshoot during optimization
  - Gradient descent will not converge easily
- The best type of divergence is steep far from the optimum, but shallow at the optimum
  - But not *too* shallow: ideally quadratic in nature

Choices for divergence





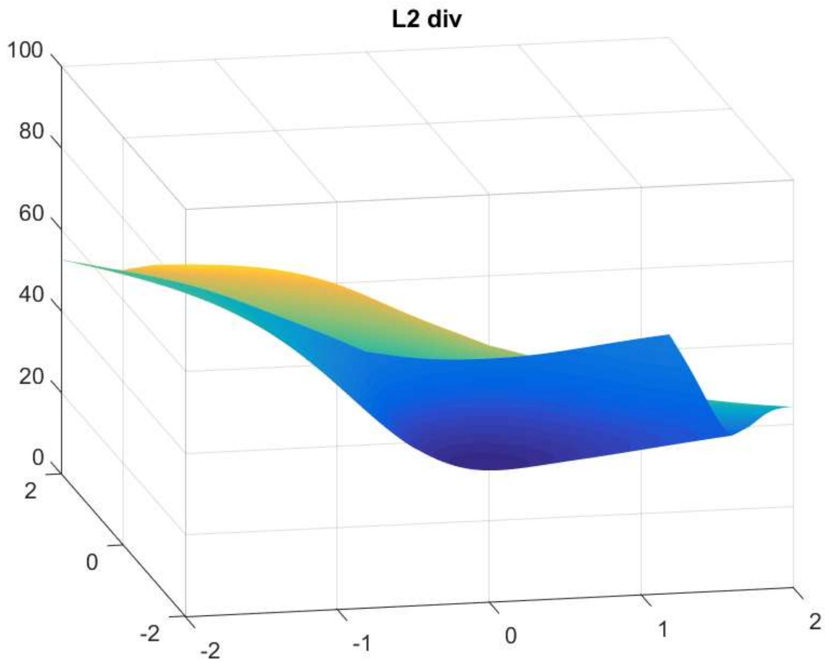
Desired output:	d	Desired output: $[0,0, \ldots, 1, \ldots, 0]$
L2	$Div = \frac{1}{2}(y-d)^2$	$Div = \frac{1}{2}\sum_i (y_i - d_i)^2$
KL	$Div = -d\log(y) - (1-d)\log(1-y)$	$Div = \sum_i d_i \log(d_i) - \sum_i d_i \log(y_i)$

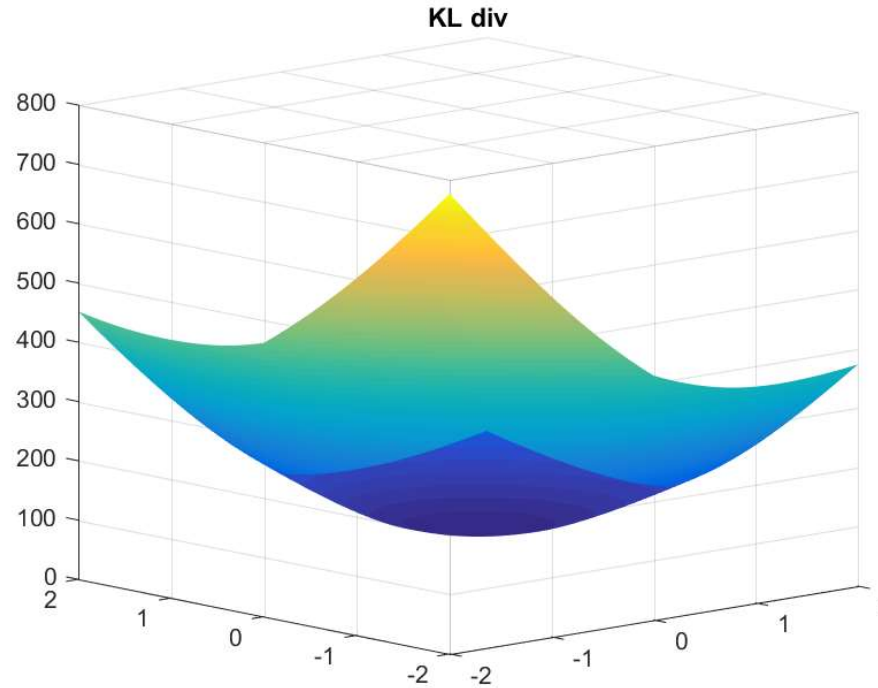
- Most common choices: The L2 divergence and the KL divergence

L2 or KL?

- The L2 divergence has long been favored in most applications
- It is particularly appropriate when attempting to perform *regression*
  - Numeric prediction
- The KL divergence is better when the intent is classification
  - The output is a probability vector

L2 or KL



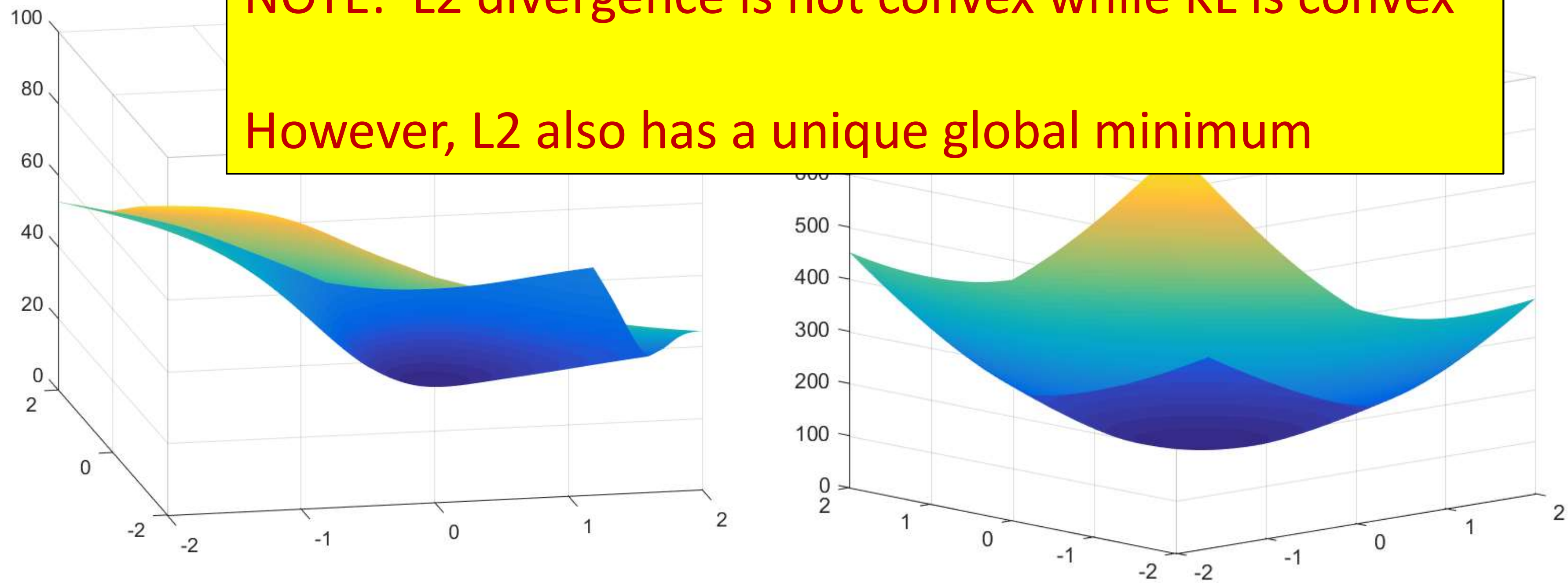


- Plot of L2 and KL divergences for a *single* perceptron, as function of weights
  - Setup: 2-dimensional input
  - 100 training examples randomly generated

L2 or KL

NOTE: L2 divergence is not convex while KL is convex

However, L2 also has a unique global minimum



- Plot of L2 and KL divergences for a *single* perceptron, as function of weights
  - Setup: 2-dimensional input
  - 100 training examples randomly generated

A note on derivatives

- Note: For L2 divergence the derivative w.r.t. the pre-activation $\boldsymbol{z}$ of the output layer is:

$$\nabla_z \frac{1}{2}\|\boldsymbol{y}-\boldsymbol{d}\|^2 = (\boldsymbol{y}-\boldsymbol{d})J_{\boldsymbol{y}}(\boldsymbol{z})$$

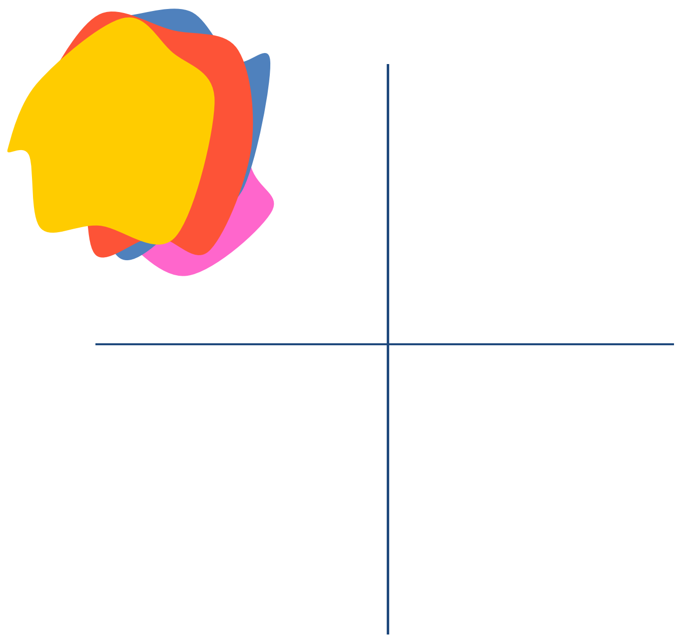
- We literally "propagate" the error $(\boldsymbol{y}-\boldsymbol{d})$ backward
  - Which is why the method is sometimes called "error backpropagation"

Story so far

- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

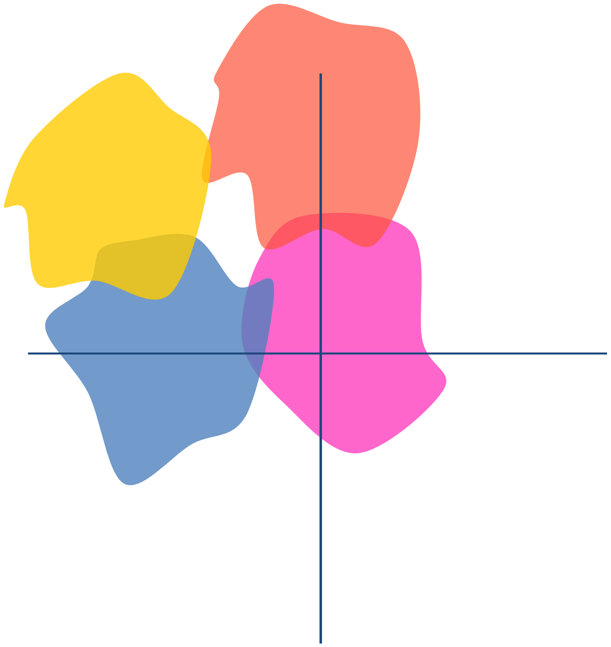
- The choice of divergence affects both the learned network and results

The problem of covariate shifts



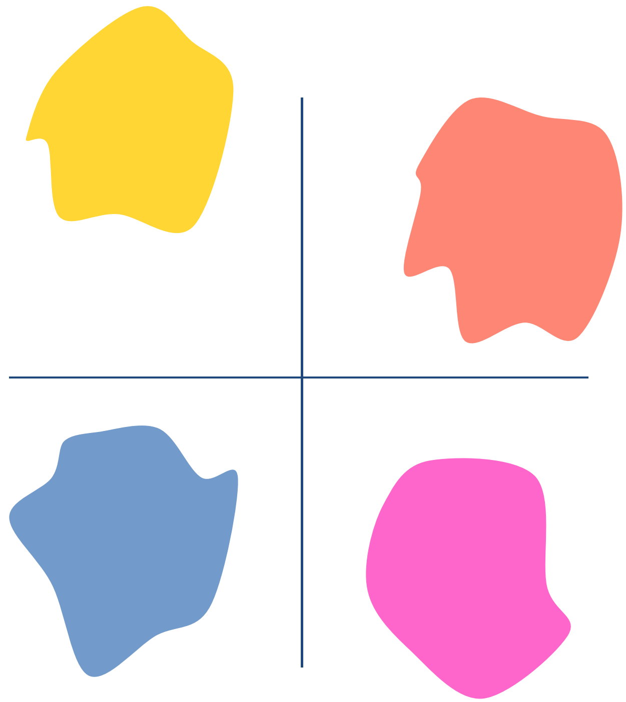
- Training assumes the training data are all similarly distributed
  - Minibatches have similar distribution

The problem of covariate shifts



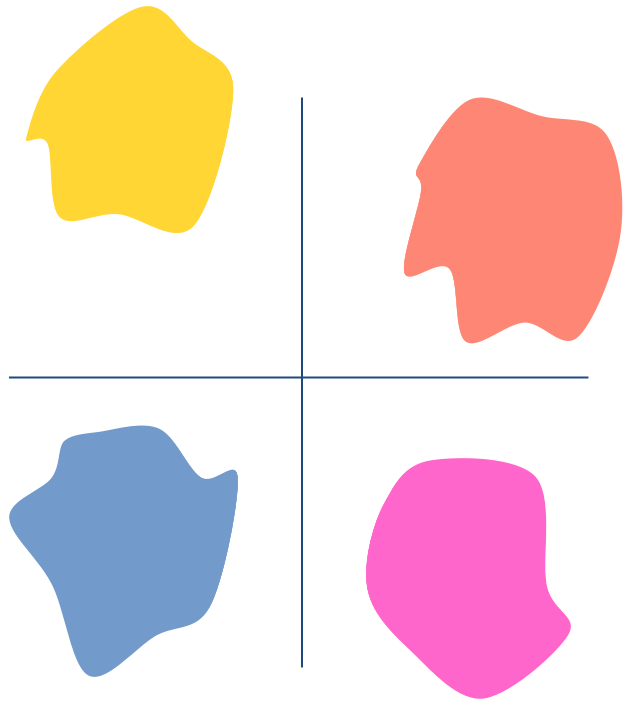
- Training assumes the training data are all similarly distributed
  - Minibatches have similar distribution
- In practice, each minibatch may have a different distribution
  - A "covariate shift"
  - Which may occur in *each* layer of the network

The problem of covariate shifts



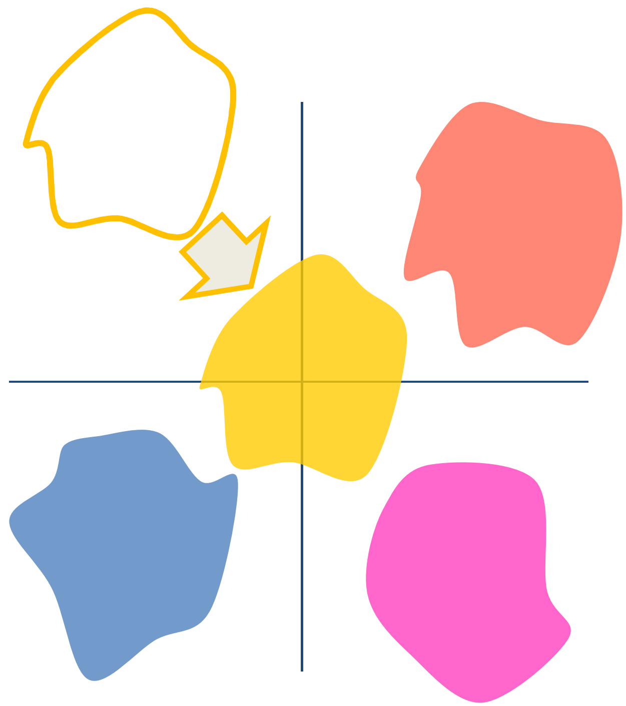
- Training assumes the training data are all similarly distributed
  - Minibatches have similar distribution
- In practice, each minibatch may have a different distribution
  - A "covariate shift"
- Covariate shifts can be large!
  - All covariate shifts can affect training badly

Solution: Move all subgroups to a "standard" location



- "Move" all batches to have a mean of 0 and unit standard deviation
  - Eliminates covariate shift between batches

Solution: Move all subgroups to a "standard" location



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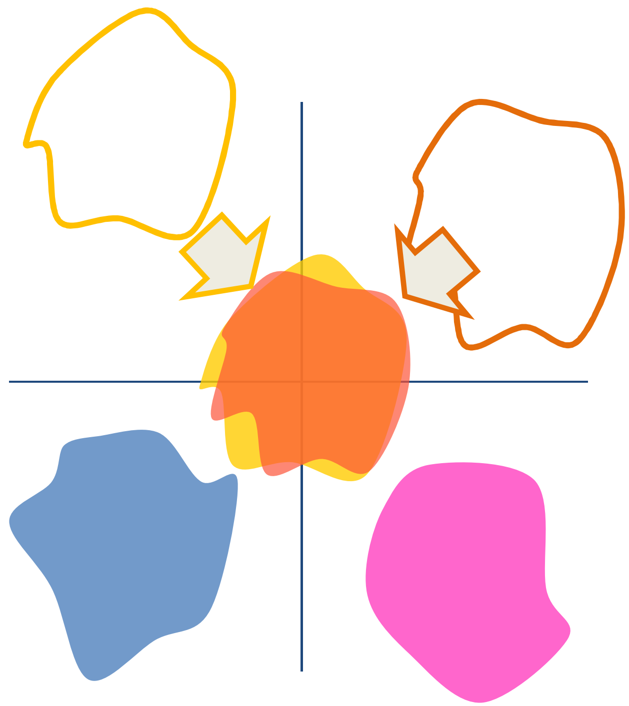

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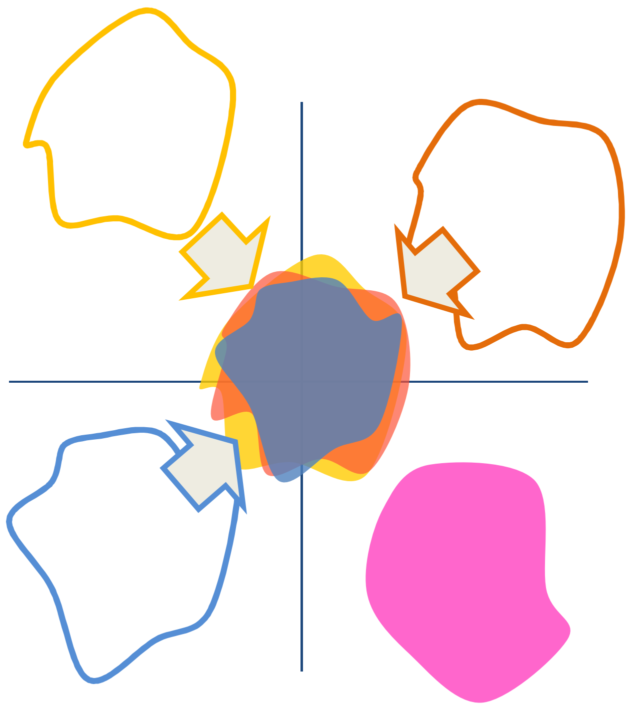

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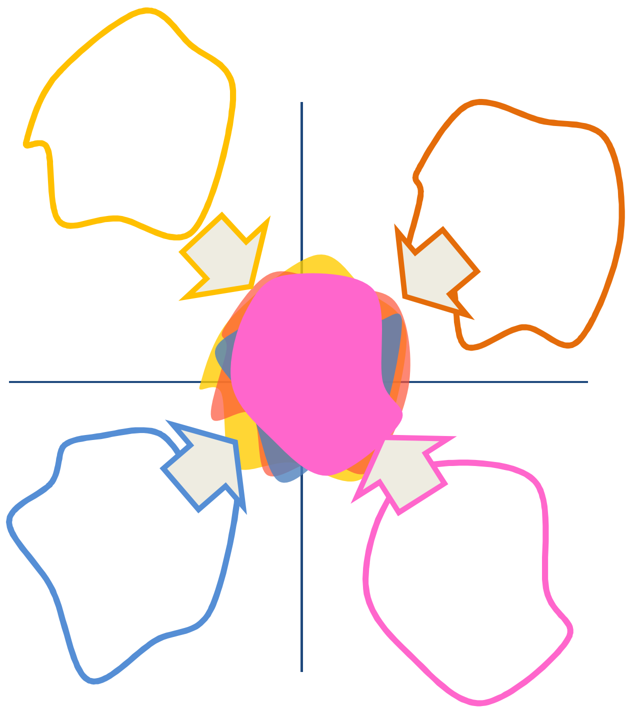

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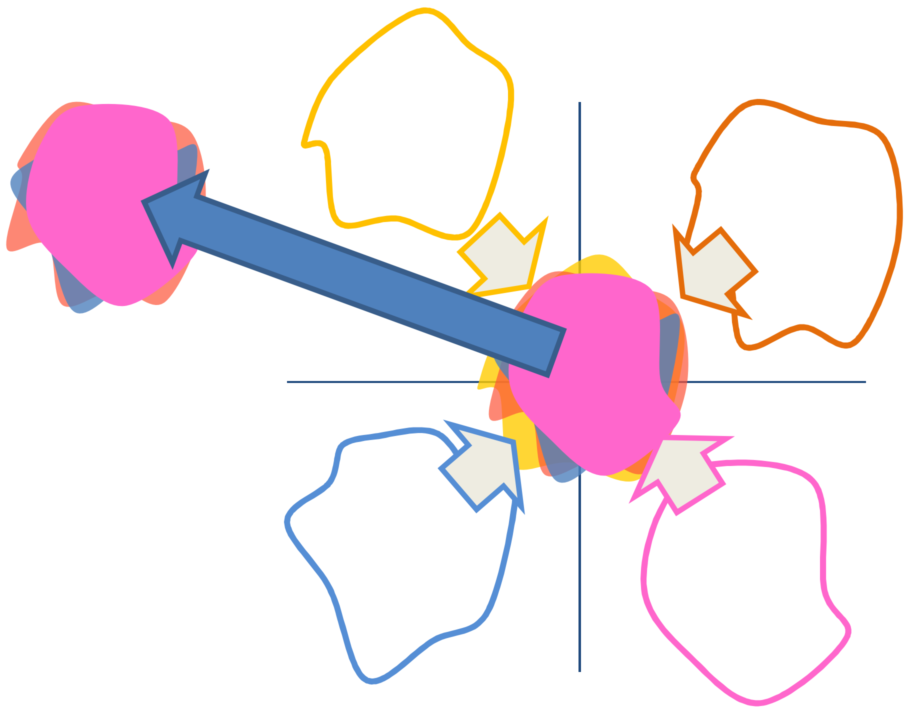
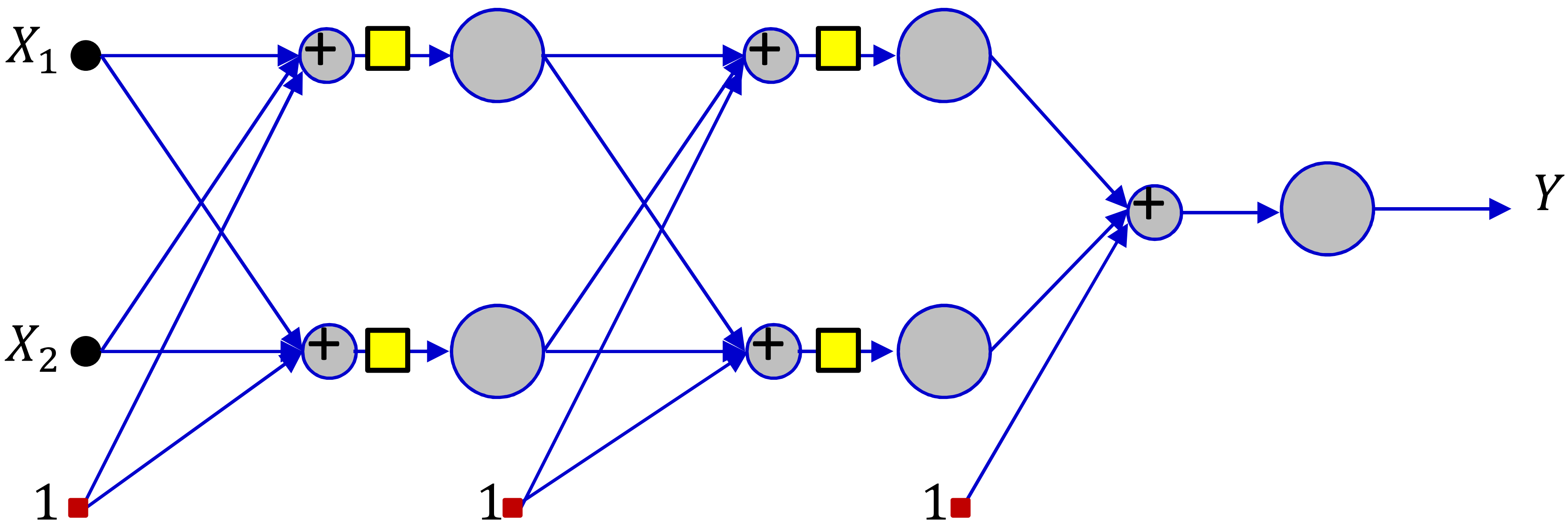


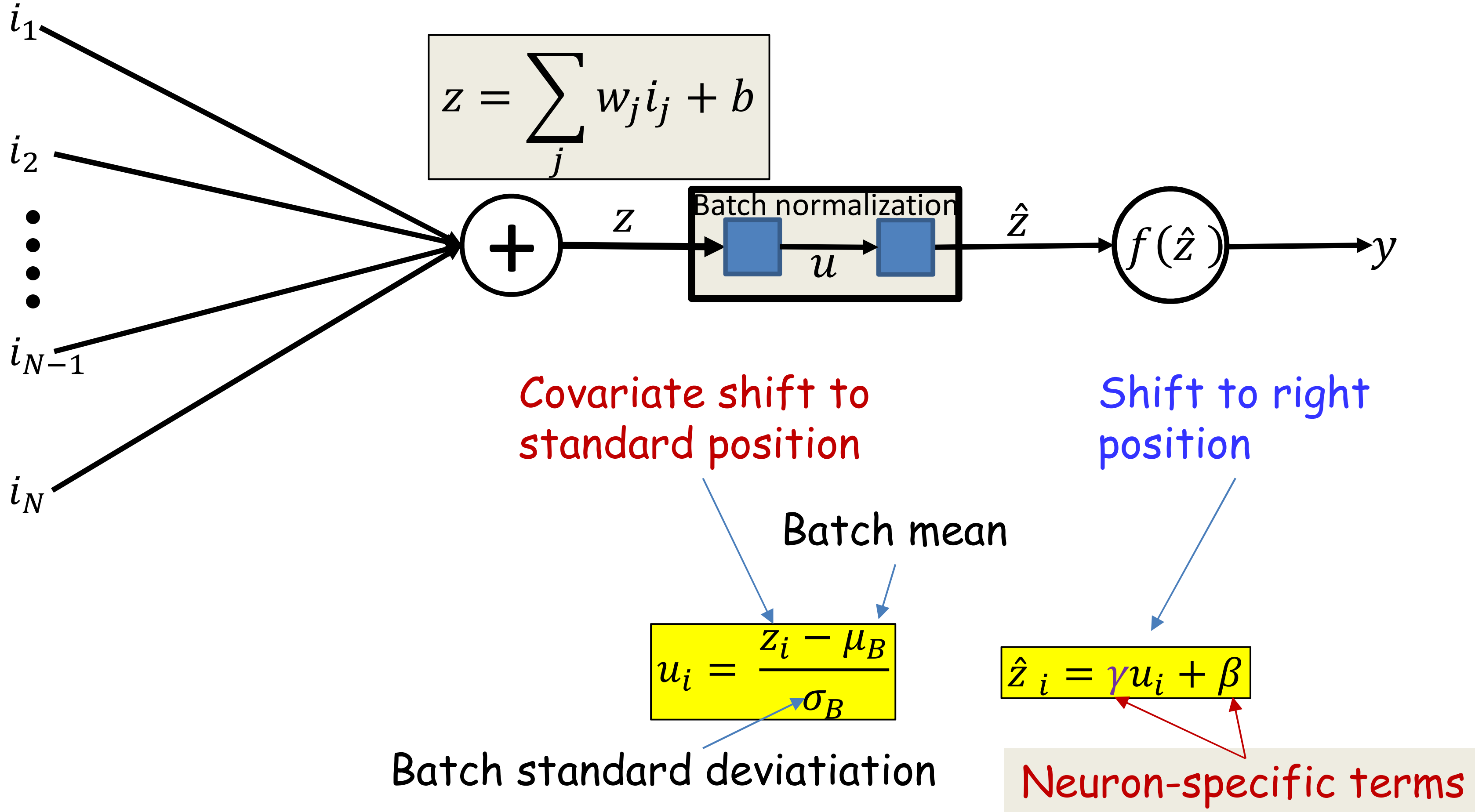
- "Move" all batches to have a mean of 0 and unit standard deviation
  - Eliminates covariate shift between batches
  - Then move the entire collection to the appropriate location

Batch normalization



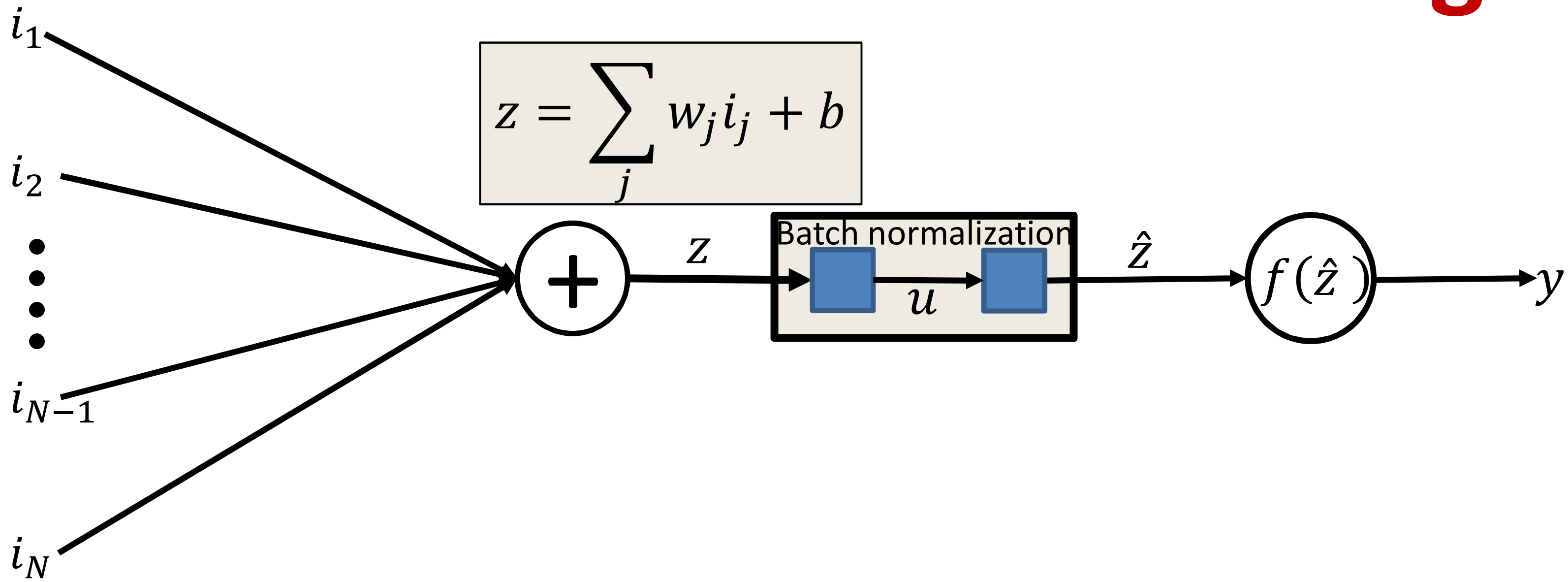
- Batch normalization is a covariate adjustment unit that happens after the weighted addition of inputs but before the application of activation
  - Is done independently for each unit, to simplify computation
- **Training: The adjustment occurs over individual minibatches**

Batch normalization



- BN aggregates the statistics over a minibatch and normalizes the batch by them
- Normalized instances are "shifted" to a *unit-specific* location

Batch normalization: Training



$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

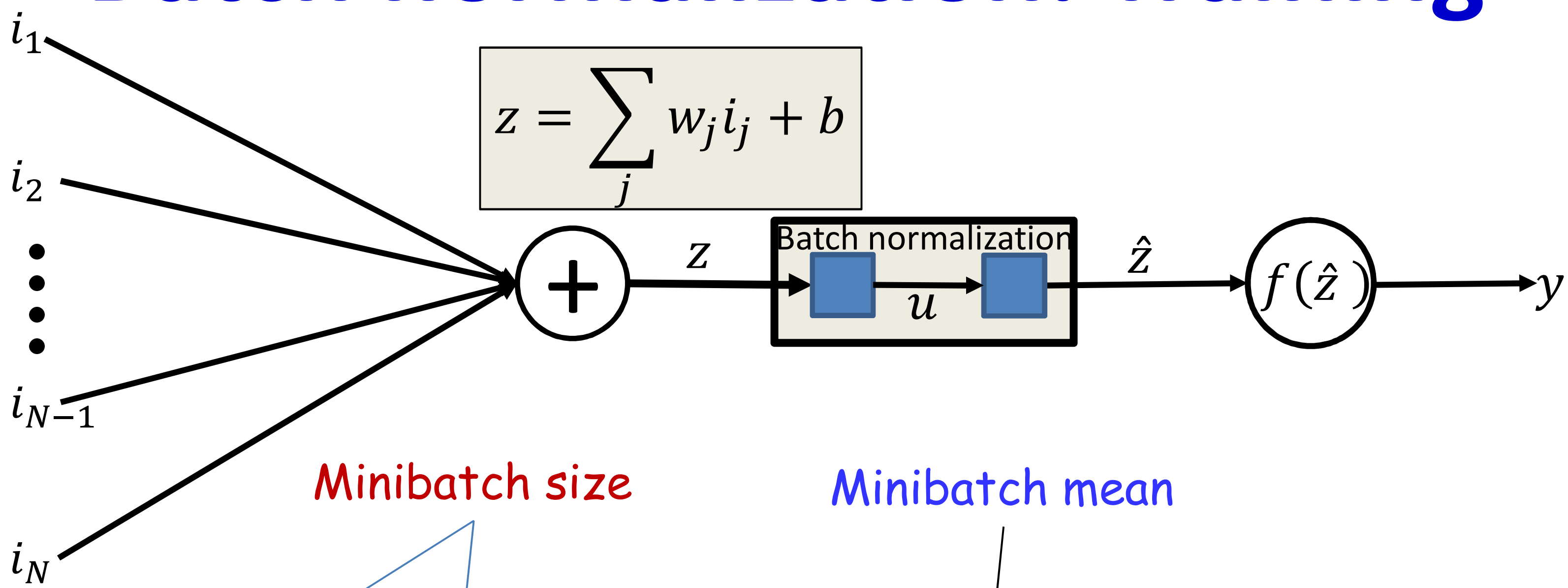
$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

- BN aggregates the statistics over a minibatch and normalizes the batch by them
- Normalized instances are “shifted” to a *unit-specific* location

Batch normalization: Training



Minibatch standard deviation

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i \qquad \sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2 \qquad u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} \qquad \hat{z}_i = \gamma u_i + \beta$$

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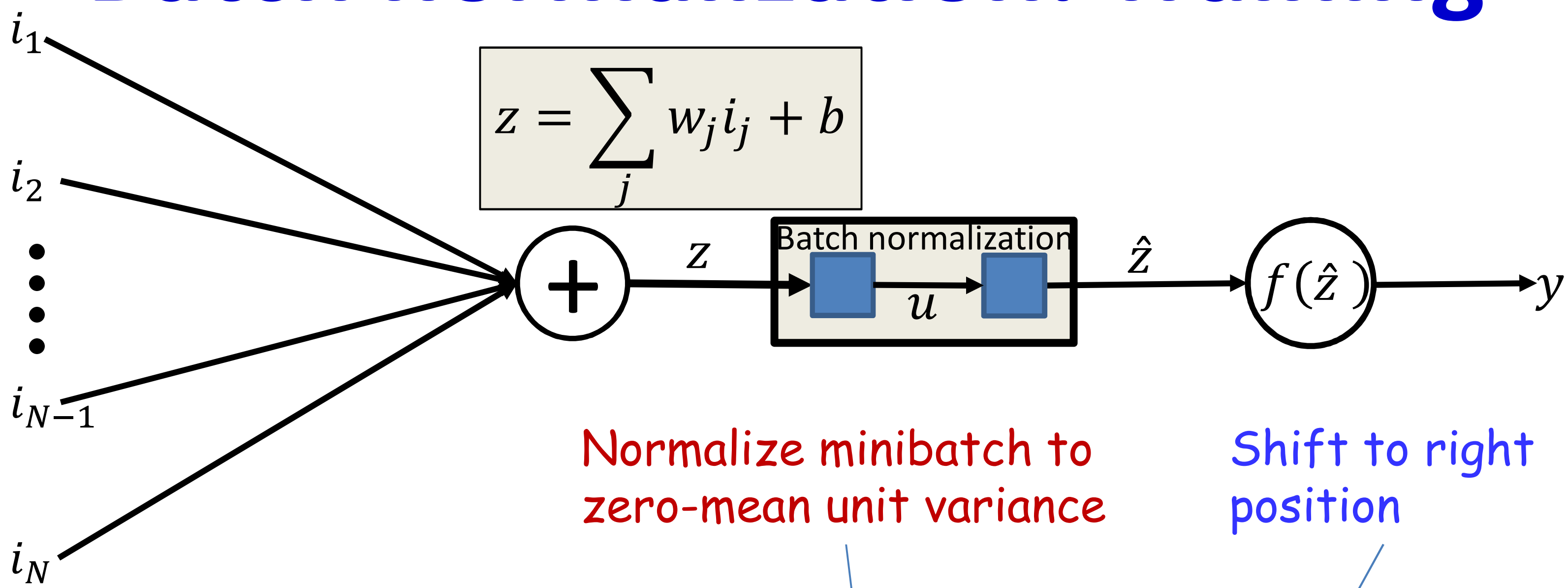
Batch normalization: Training



$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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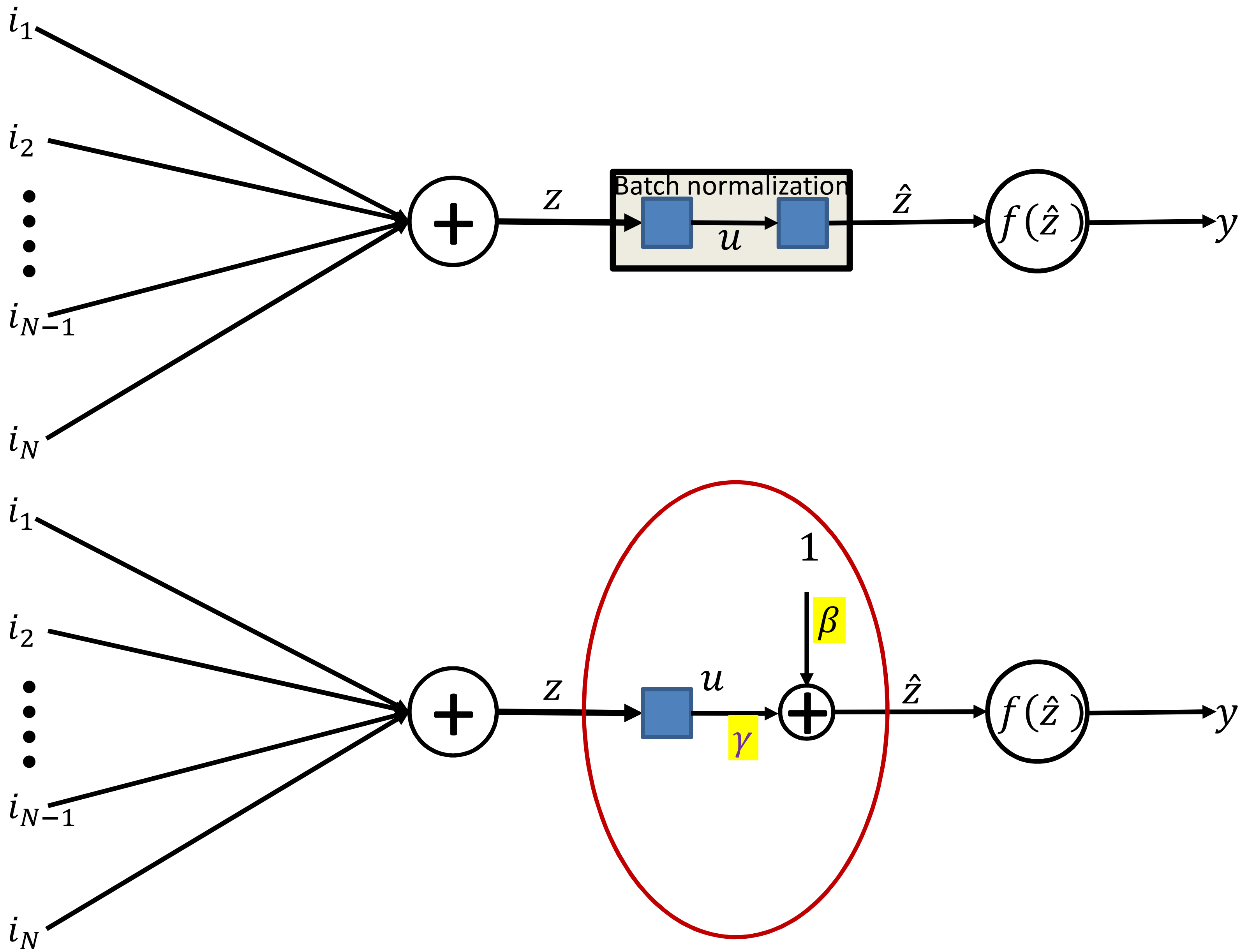
$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

- BN aggregates the statistics over a minibatch and normalizes the batch by them
- Normalized instances are "shifted" to a *unit-specific* location

A better picture for batch norm



A note on derivatives

- In conventional learning, we attempt to compute the derivative of the divergence for *individual* training instances w.r.t. parameters

- This is based on the following relations

$$Div(minibatch) = \frac{1}{B}\sum_t Div(Y_t(X_t), d_t(X_t))$$

$$\frac{dDiv(minibatch)}{dw_{i,j}^{(k)}} = \frac{1}{T}\sum_t \frac{dDiv(Y_t(X_t), d_t(X_t))}{dw_{i,j}^{(k)}}$$

- If we use Batch Norm, the above relation gets a little complicated

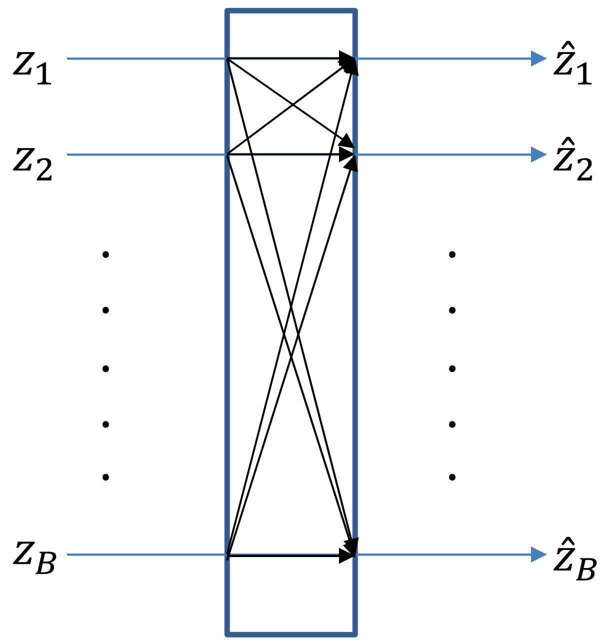
A note on derivatives

- The outputs are now functions of μ_B and σ_B^2 which are functions of the entire minibatch

$$Div(MB) = \frac{1}{B}\sum_t Div(Y_t(X_t, \mu_B, \sigma_B^2), d_t(X_t))$$

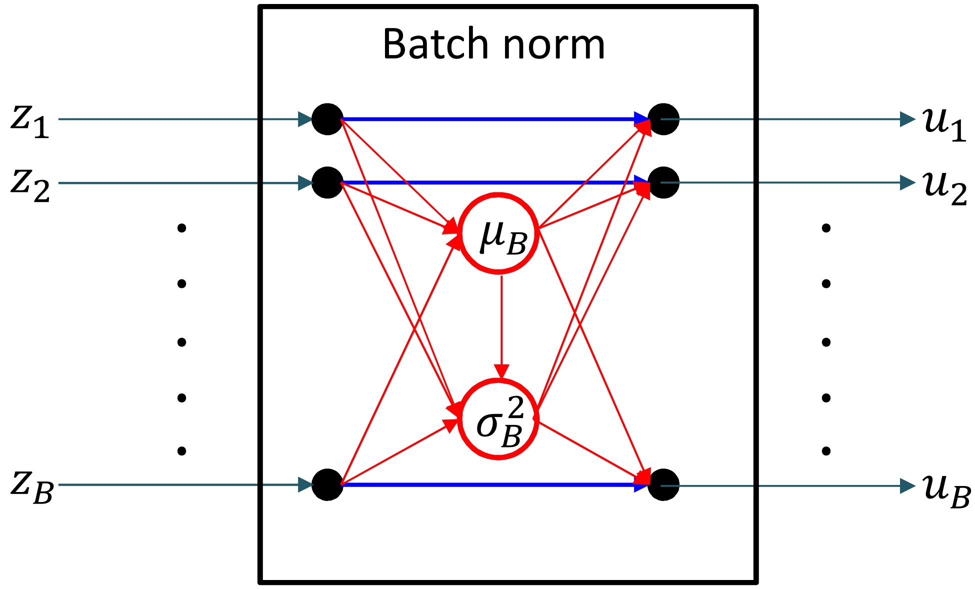
- The Divergence for each Y_t depends on *all* the X_t within the minibatch
- Specifically, within each layer, we get the relationship in the following slide

Batchnorm is a vector function over the minibatch



- Batch normalization is really a *vector* function applied over all the inputs from a minibatch
  - Every z_i affects every $\hat{z}_j$
  - Shown on the next slide
- To compute the derivative of the divergence w.r.t any z_i, we must consider all $\hat{z}_j s$ in the batch

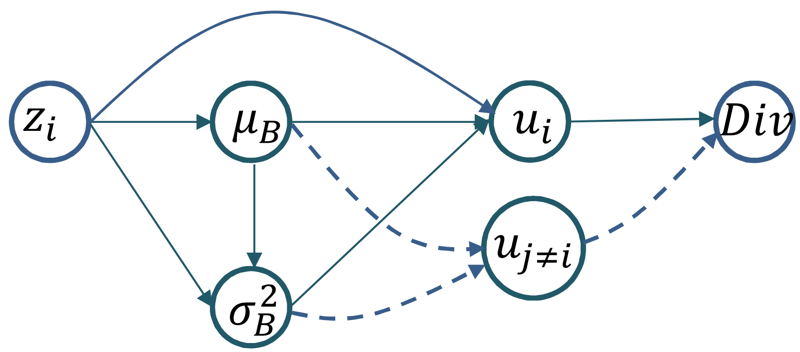
Batchnorm



- The complete dependency figure for Batchnorm
- Note : inputs and outputs are different *instances* in a minibatch
  - The diagram represents BN occurring at a *single neuron*
- You can use vector function differentiation rules to compute the derivatives
  - But the equations in the following slides summarize them for you
  - The actual derivation uses the simplified diagram shown in the next slide, but you could do it directly off the figure above and arrive at the same answers

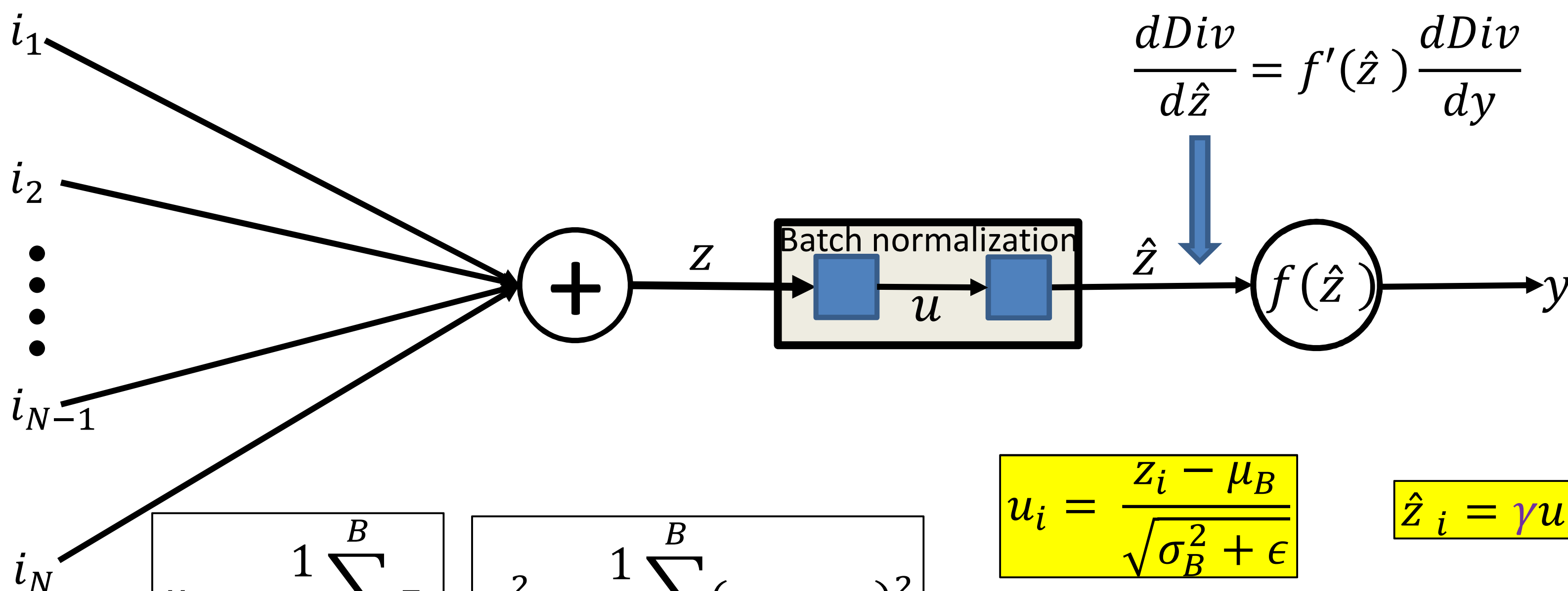
Batchnorm

Influence diagram



- Simplified diagram for a *single* input in a minibatch

Batch normalization: Backpropagation



$$\frac{dDiv}{d\hat{z}} = f'(\hat{z})\frac{dDiv}{dy}$$

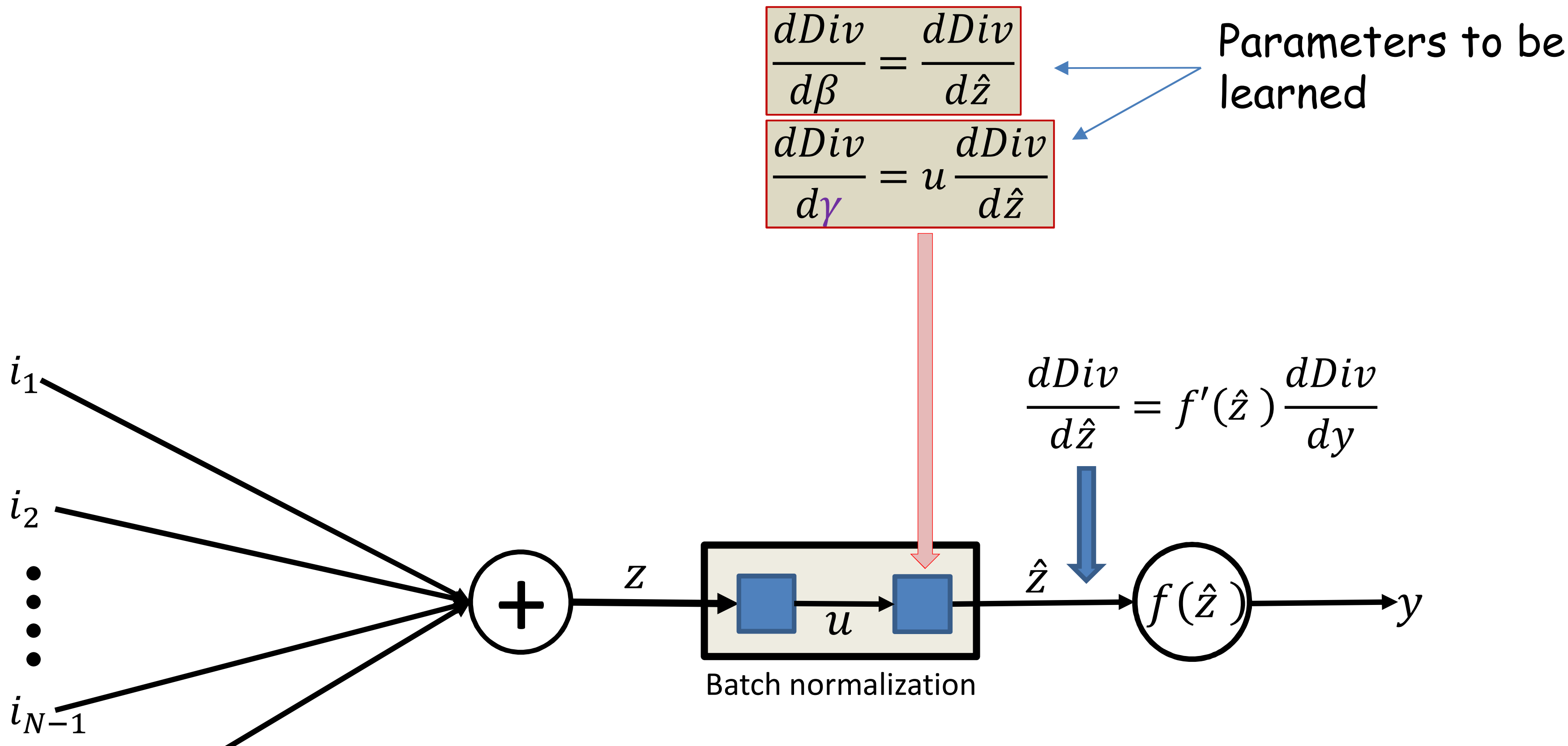
$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

Batch normalization: Backpropagation



$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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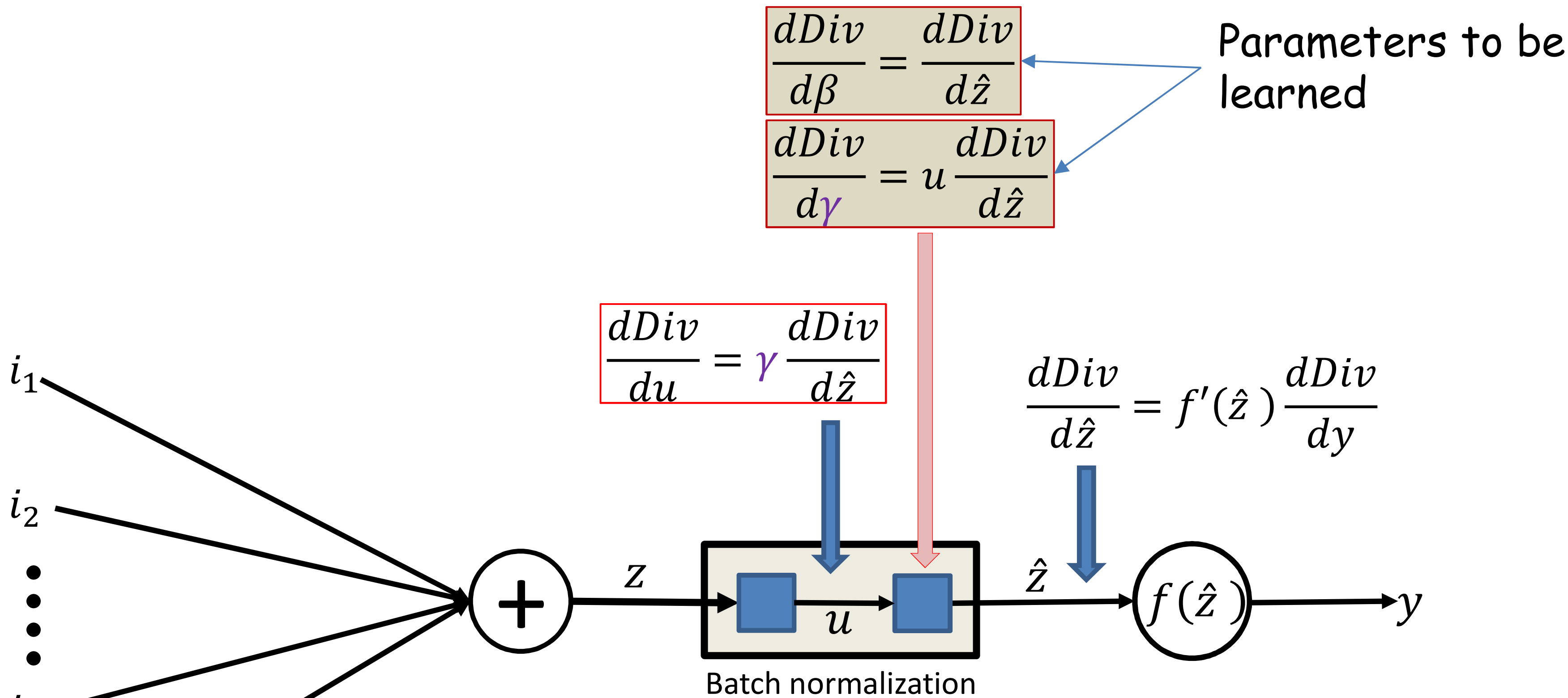
$$\hat{z}_i = \gamma u_i + \beta$$

Batch normalization: Backpropagation



$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

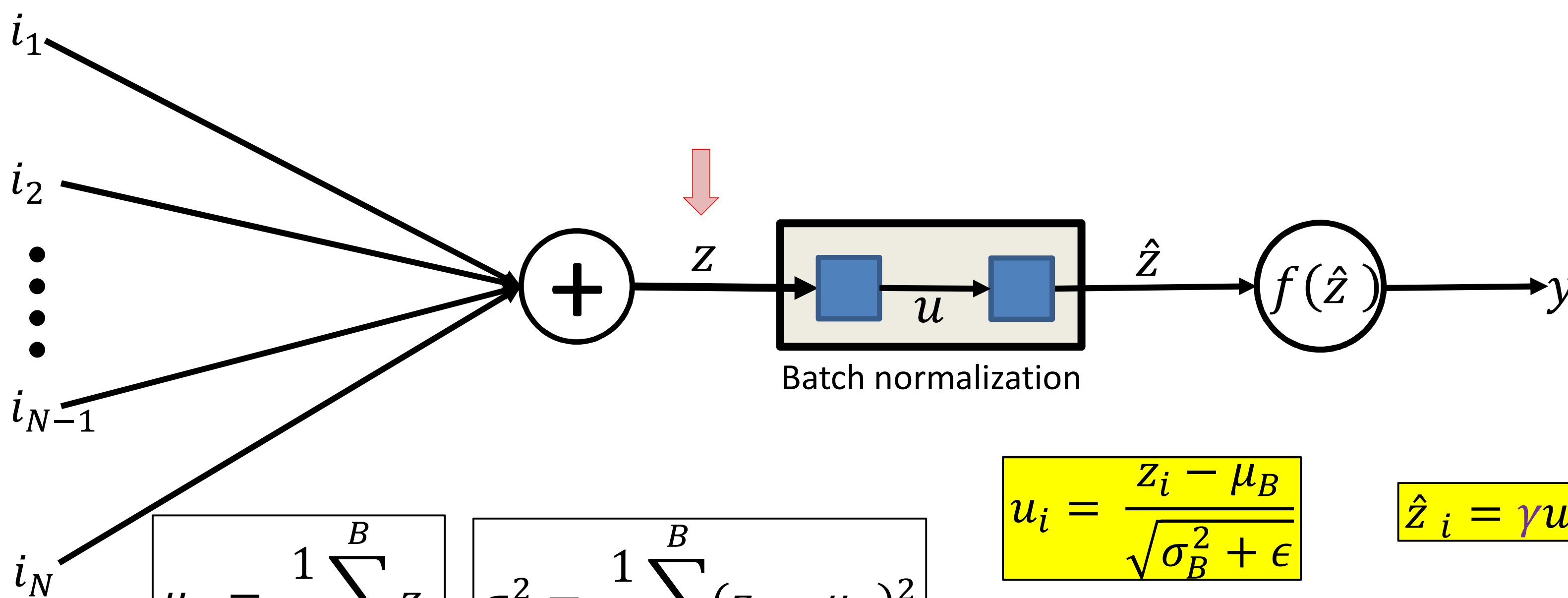
$$\hat{z}_i = \gamma u_i + \beta$$

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

Batch normalization: Backpropagation

- Final step of backprop: compute $\frac{\partial Div}{\partial z_i}$



$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

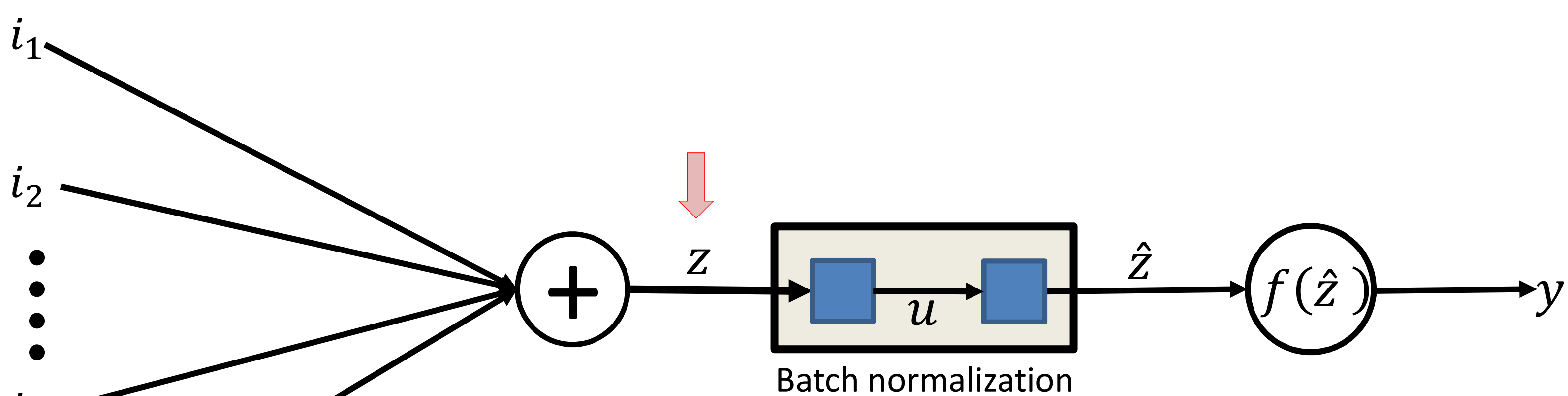
$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

Batch normalization: Backpropagation

$$Div = function(u_i, \mu_B, \sigma_B^2)$$

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{\partial \mu_B}{\partial z_i}$$



$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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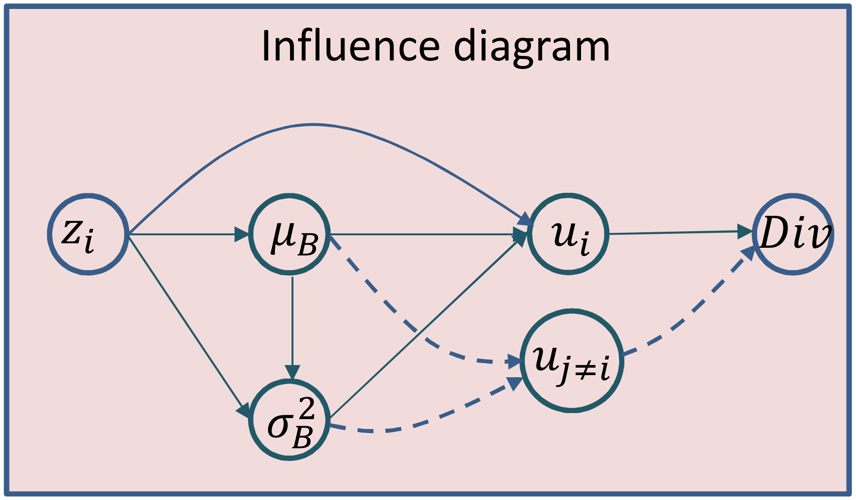
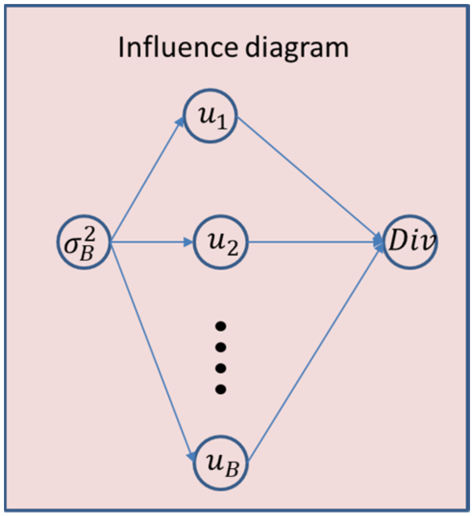
Batch normalization: Backpropagation

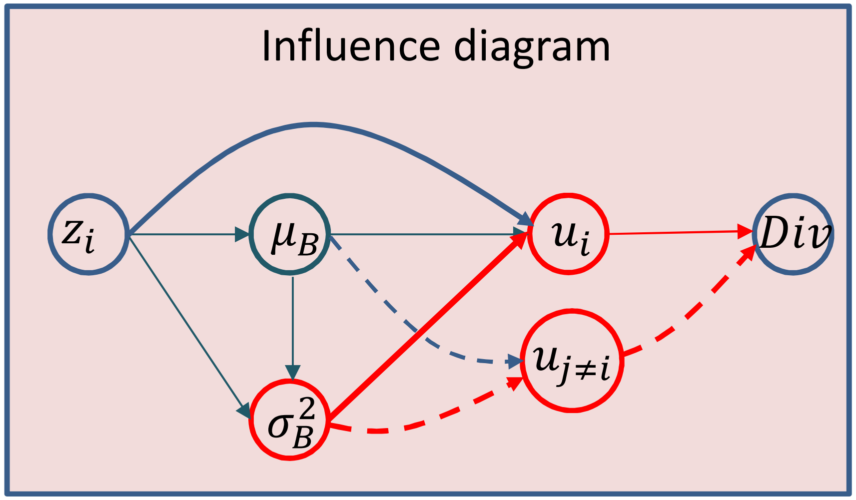


Dotted lines show dependence through other u_js because Divergence is computed over a minibatch

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{\partial \mu_B}{\partial z_i}$$

Batch normalization: Backpropagation





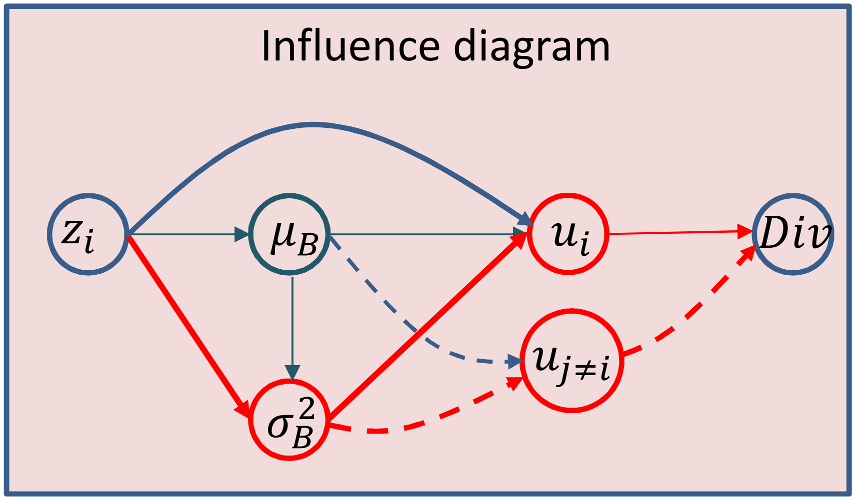
Dotted lines show dependence through other u_js because Divergence is computed over a minibatch

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{\partial \mu_B}{\partial z_i}$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\frac{\partial Div}{\partial \sigma_B^2} = \frac{-1}{2}(\sigma_B^2 + \epsilon)^{-3/2} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}(z_i - \mu_B)$$

Batch normalization: Backpropagation



Dotted lines show dependence through other u_js because Divergence is computed over a minibatch

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{\partial \mu_B}{\partial z_i}$$

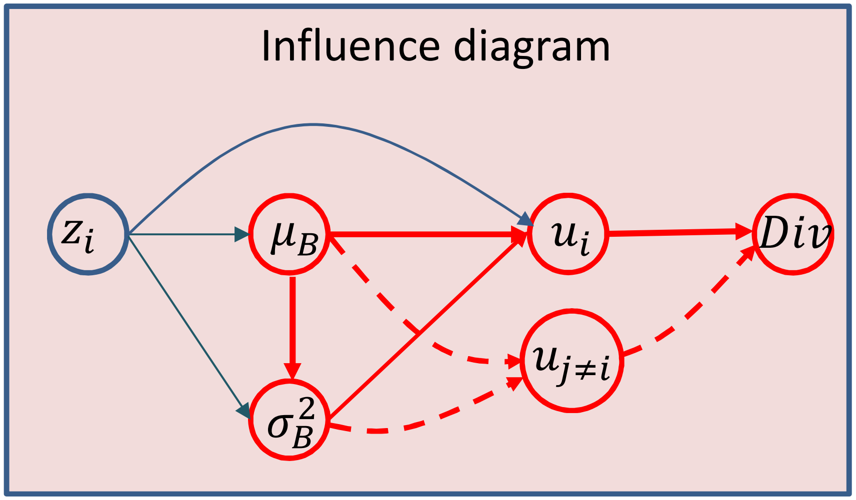
$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\frac{\partial Div}{\partial \sigma_B^2} = \frac{-1}{2}\left(\sigma_B^2 + \epsilon\right)^{-3/2} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}(z_i - \mu_B)$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

$$\frac{\partial \sigma_B^2}{\partial z_i} = \frac{2(z_i - \mu_B)}{B}$$

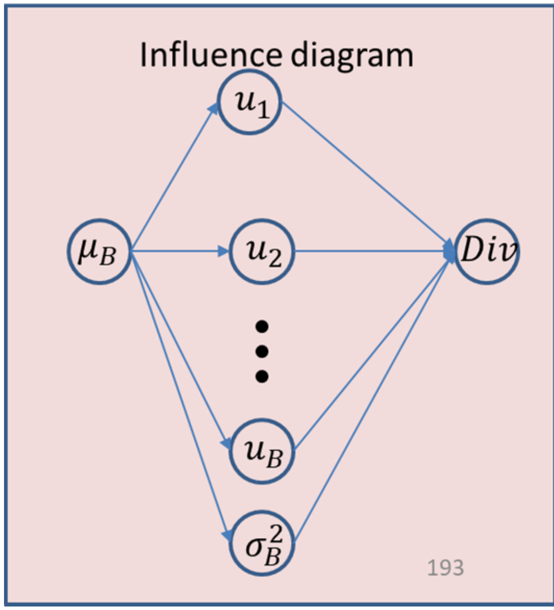
Batch normalization: Backpropagation

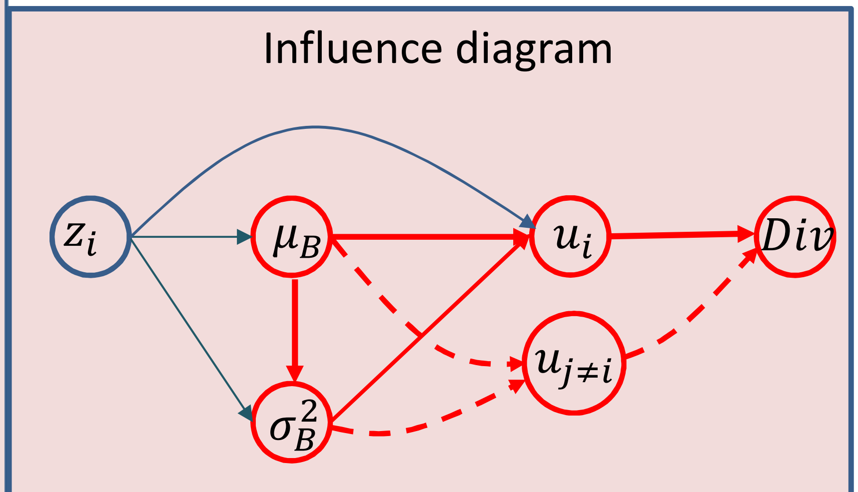


Dotted lines show dependence through other u_js because Divergence is computed over a minibatch

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{\partial \mu_B}{\partial z_i}$$

Batch normalization: Backpropagation





Dotted lines show dependence through other u_js because Divergence is computed over a minibatch

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i}\cdot\frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2}\cdot\frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B}\cdot\frac{\partial \mu_B}{\partial z_i}$$

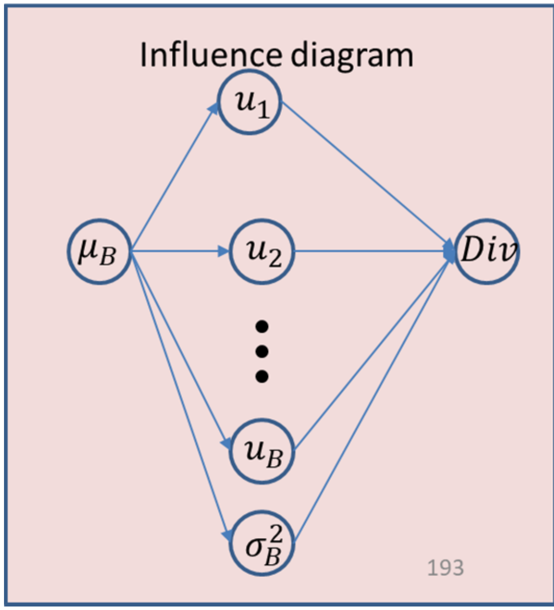
Second term goes to 0

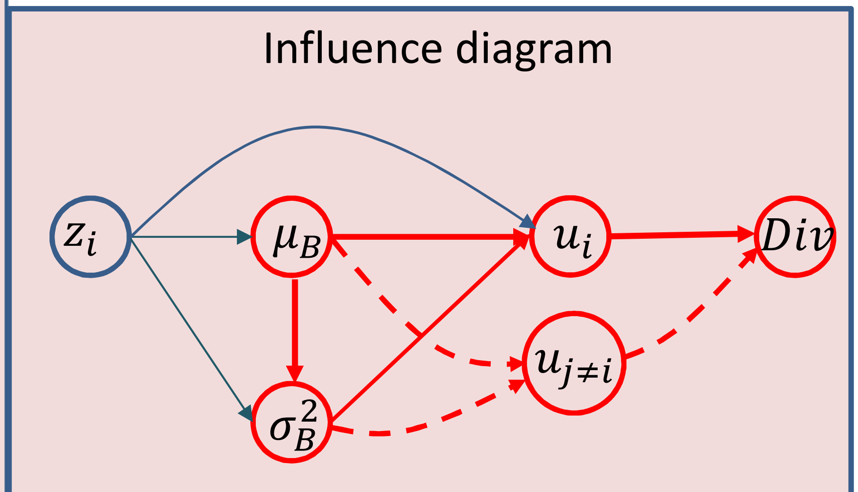
$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\frac{\partial Div}{\partial \mu_B} = \left(\sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}\cdot\frac{-1}{\sqrt{\sigma_B^2 + \epsilon}}\right) + \frac{\partial Div}{\partial \sigma_B^2}\cdot\frac{\sum_{i=1}^{B} -2(z_i - \mu_B)}{B}$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

Batch normalization: Backpropagation





Dotted lines show dependence through other u_js because Divergence is computed over a minibatch

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{\partial \mu_B}{\partial z_i}$$

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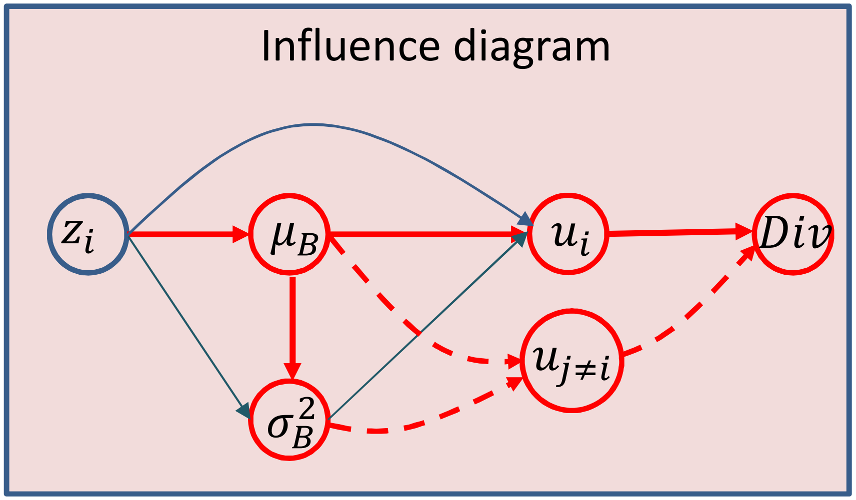
$$\frac{\partial Div}{\partial \mu_B} = \frac{-1}{\sqrt{\sigma_B^2 + \epsilon}} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

$$\sigma_B^2 = \frac{1}{B} \sum_{i=1}^{B} (z_i - \mu_B)^2$$

Batch normalization: Backpropagation



Dotted lines show dependence through other u_js because Divergence is computed over a minibatch

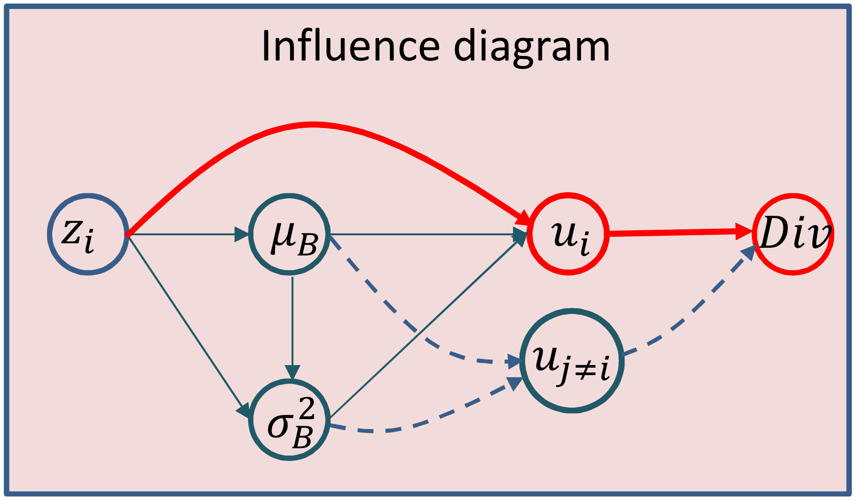
$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{\partial u_i}{\partial z_i} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{\partial \mu_B}{\partial z_i}$$

$$\frac{\partial \mu_B}{\partial z_i} = \frac{1}{B}$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\frac{\partial Div}{\partial \mu_B} = \frac{-1}{\sqrt{\sigma_B^2 + \epsilon}} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

Batch normalization: Backpropagation



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$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

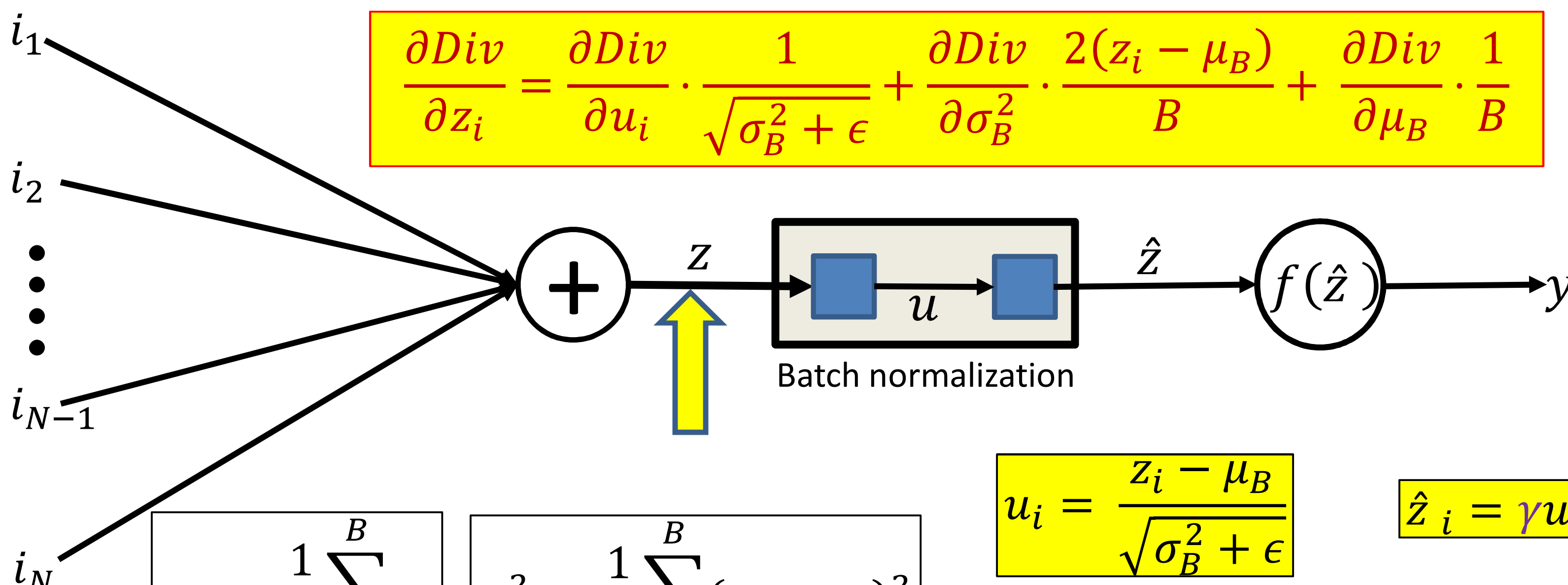
$$\frac{\partial Div}{\partial u_i} \cdot \frac{1}{\sqrt{\sigma_B^2 + \epsilon}}$$

Batch normalization: Backpropagation

$$\frac{\partial Div}{\partial \sigma_B^2} = \frac{-1}{2}\left(\sigma_B^2 + \epsilon\right)^{-3/2} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}\left(z_i - \mu_B\right)$$

$$\frac{\partial Div}{\partial \mu_B} = \frac{-1}{\sqrt{\sigma_B^2 + \epsilon}} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{2(z_i - \mu_B)}{B} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{1}{B}$$



$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

$$\mu_B = \frac{1}{B} \sum_{i=1}^{B} z_i$$

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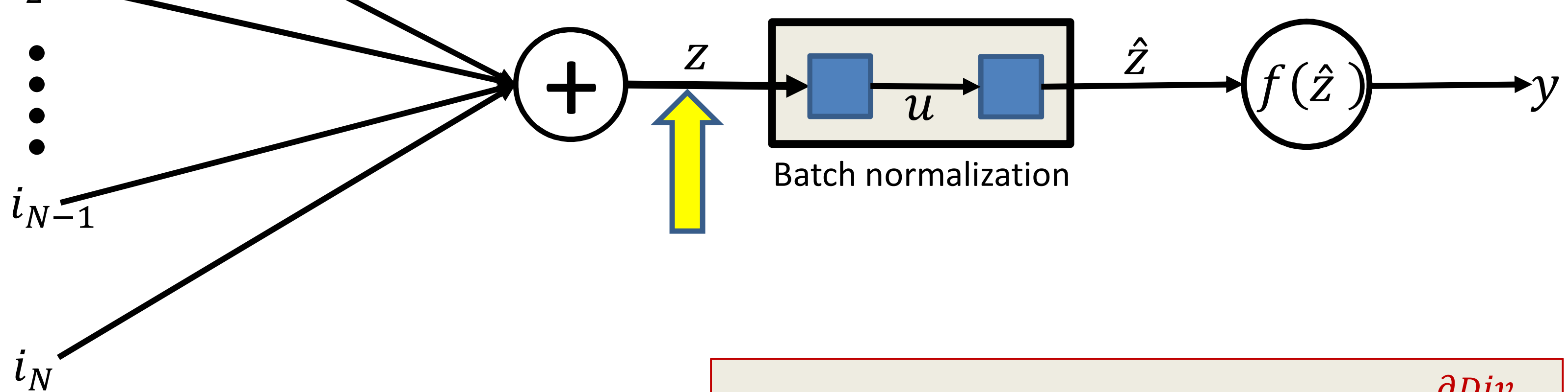
Batch normalization: Backpropagation

$$\frac{\partial Div}{\partial \sigma_B^2} = \frac{-1}{2}(\sigma_B^2 + \epsilon)^{-3/2} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}(z_i - \mu_B)$$

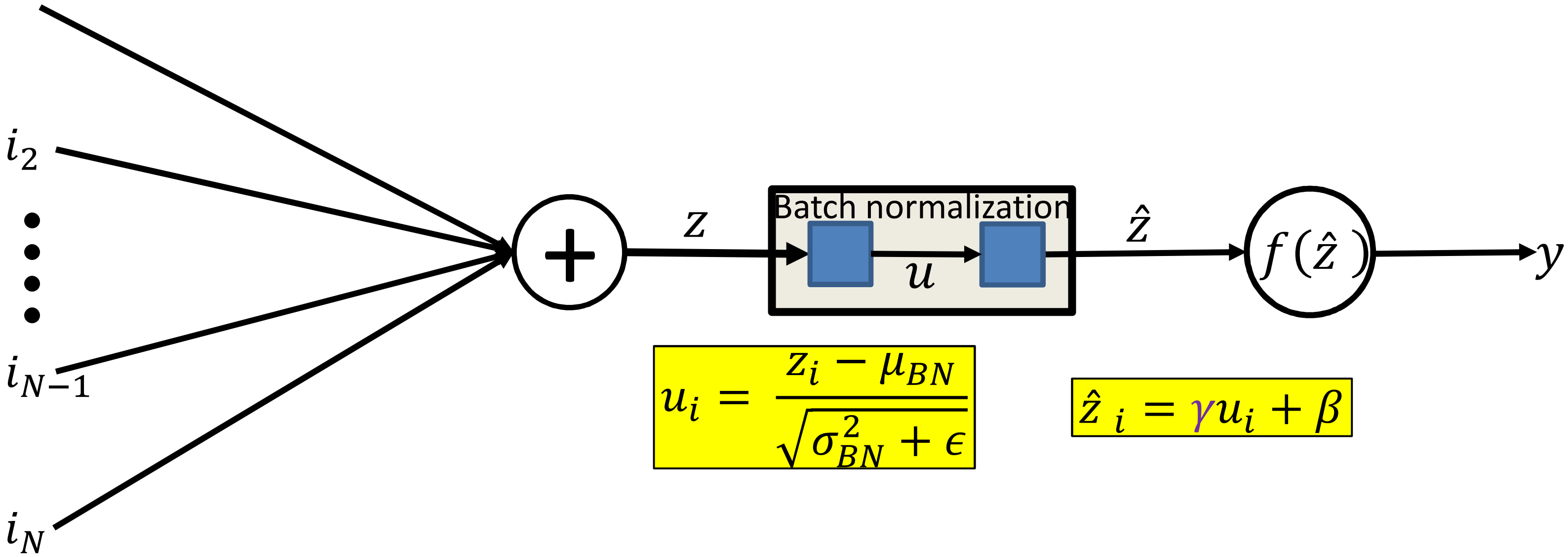
$$\frac{\partial Div}{\partial \mu_B} = \frac{-1}{\sqrt{\sigma_B^2 + \epsilon}} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{2(z_i - \mu_B)}{B} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{1}{B}$$



The rest of backprop continues from $\frac{\partial Div}{\partial z_i}$

Batch normalization: Inference



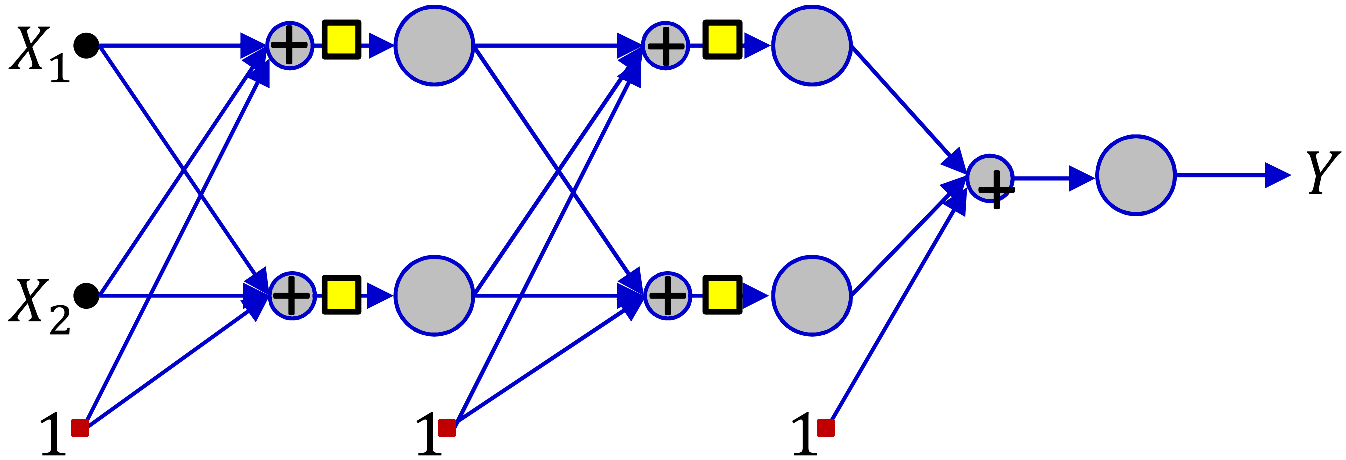
- On test data, BN requires μ_B and σ_B^2.
- We will use the *average over all training minibatches*

$$\mu_{BN} = \frac{1}{Nbatches} \sum_{batch} \mu_B(batch)$$

$$\sigma_{BN}^2 = \frac{B}{(B-1)Nbatches} \sum_{batch} \sigma_B^2(batch)$$

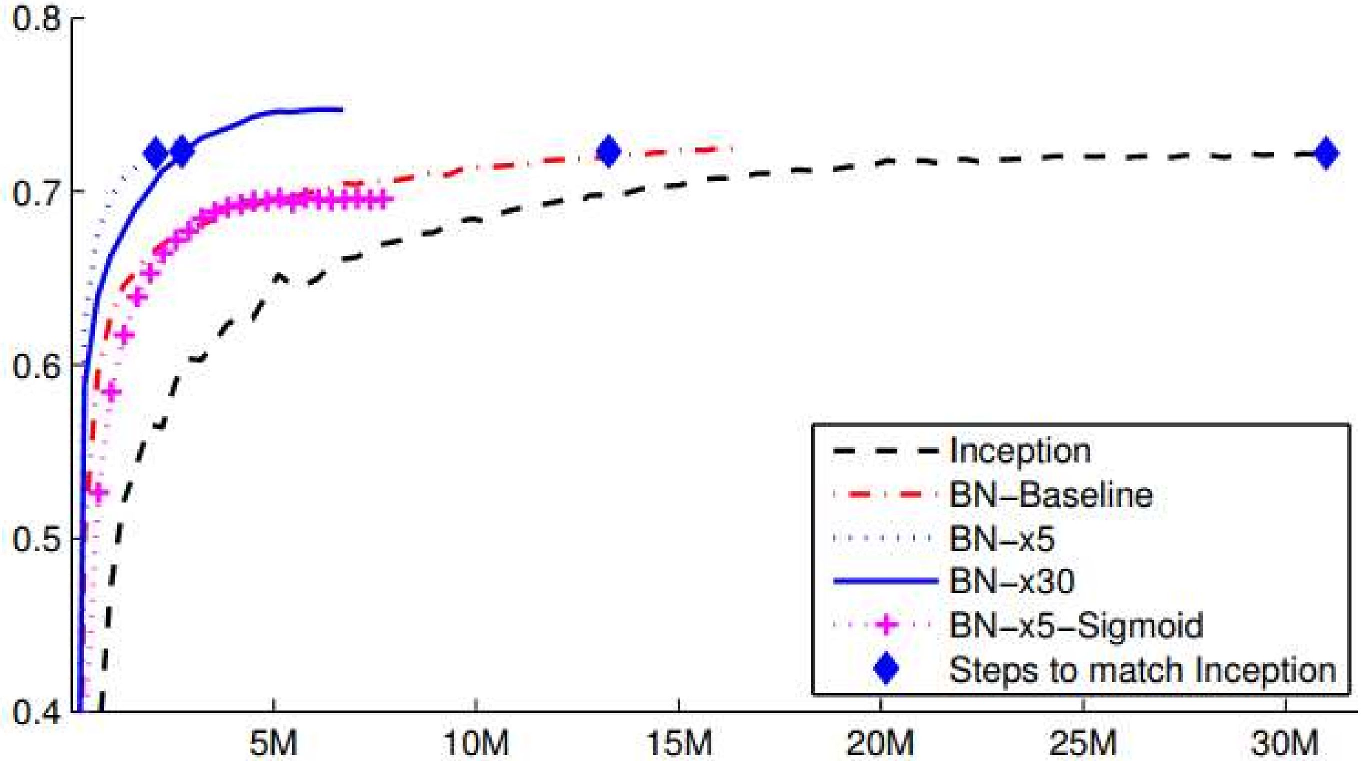
- Note: these are *neuron-specific*
  - $\mu_B(batch)$ and $\sigma_B^2(batch)$ here are obtained from the *final converged network*
  - The $B/(B-1)$ term gives us an unbiased estimator for the variance

Batch normalization



- Batch normalization may only be applied to *some* layers
  - Or even only selected neurons in the layer
- Improves both convergence rate and neural network performance
  - Anecdotal evidence that BN eliminates the need for dropout
  - To get maximum benefit from BN, learning rates must be increased and learning rate decay can be faster
    - Since the data generally remain in the high-gradient regions of the activations
  - Also needs better randomization of training data order

Batch Normalization: Typical result



- Performance on Imagenet, from Ioffe and Szegedy, JMLR 2015

Story so far

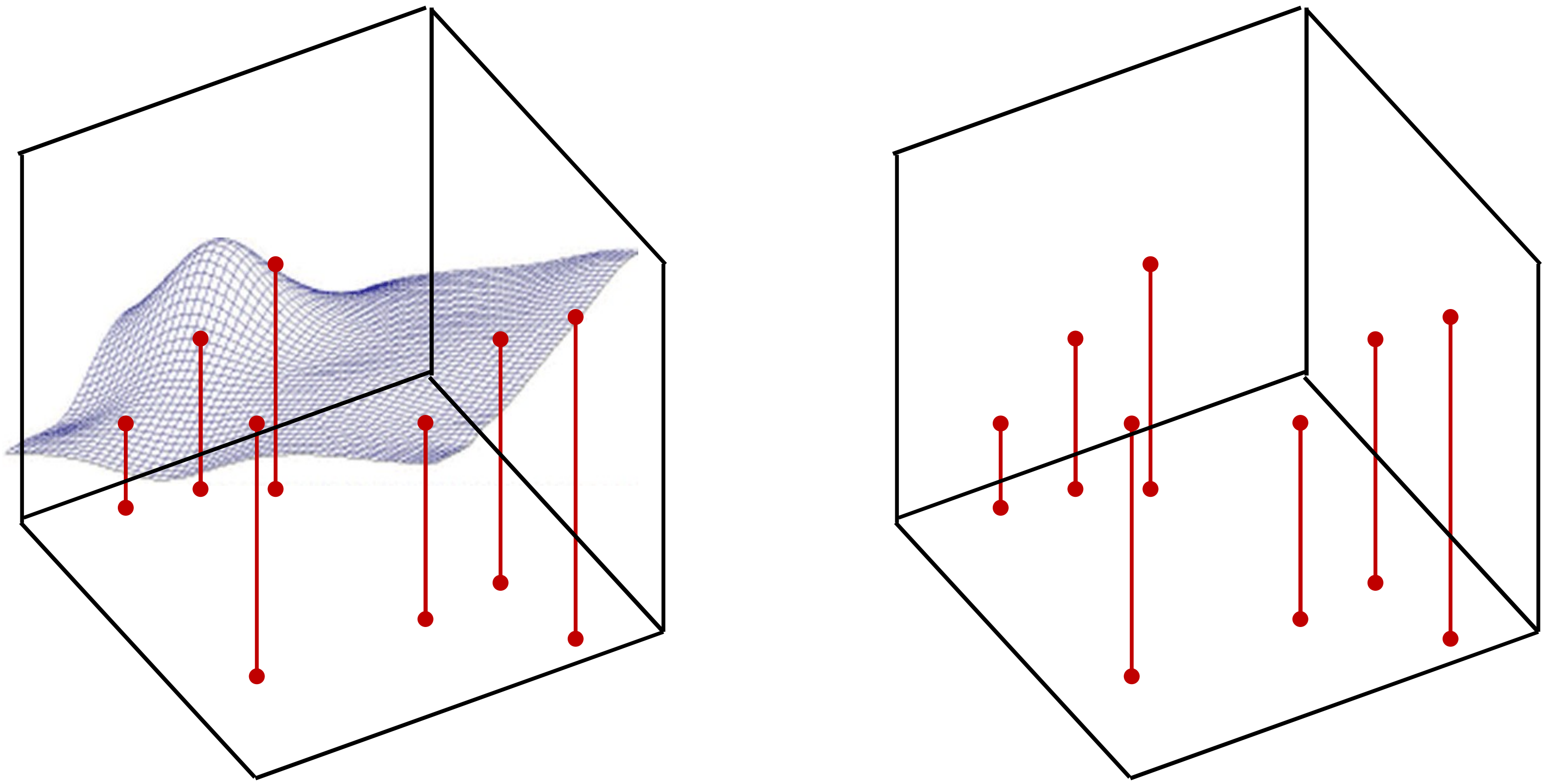
- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

- The choice of divergence affects both the learned network and results
- Covariate shift between training and test may cause problems and may be handled by batch normalization

The problem of data underspecification

- The figures shown to illustrate the learning problem so far were *fake news*..

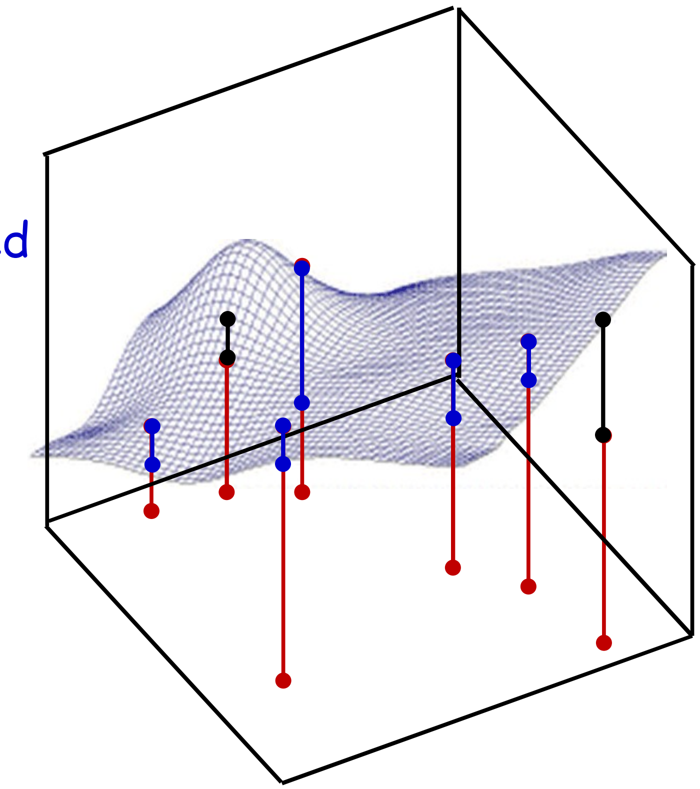
Learning the network



- We attempt to learn an entire function from just a few *snapshots* of it

General approach to training

Blue lines: error when function is *below* desired output

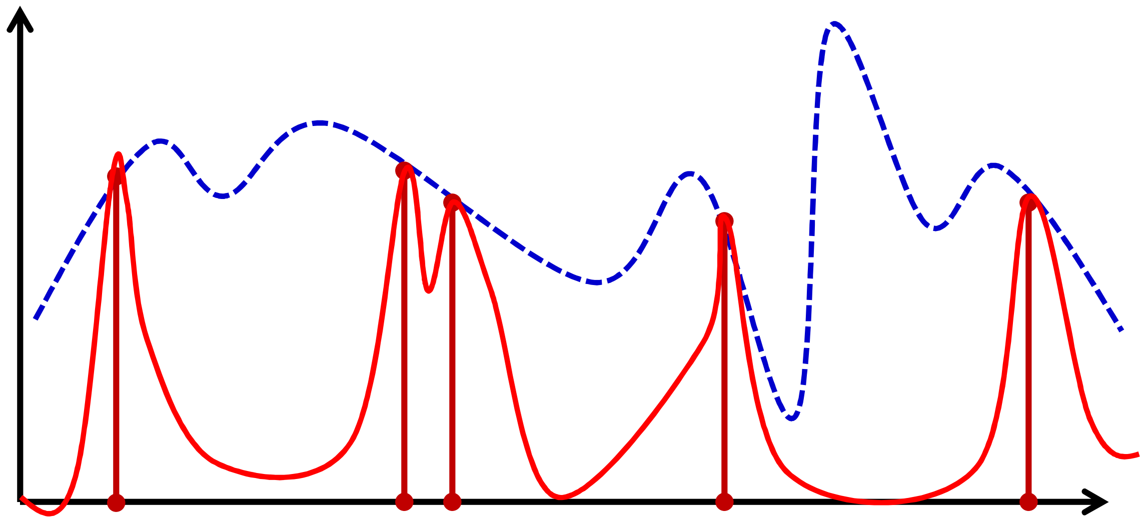


Black lines: error when function is *above* desired output

$$E = \sum_i (y_i - f(\mathbf{x}_i, \mathbf{W}))^2$$

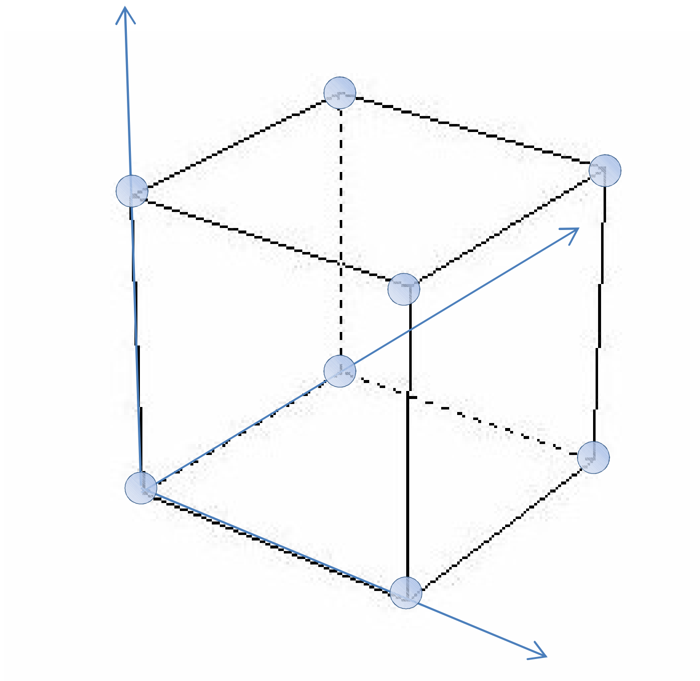
- Define an *error* between the ***actual*** network output for any parameter value and the *desired* output
  - Error typically defined as the *sum* of the squared error over individual training instances

Overfitting



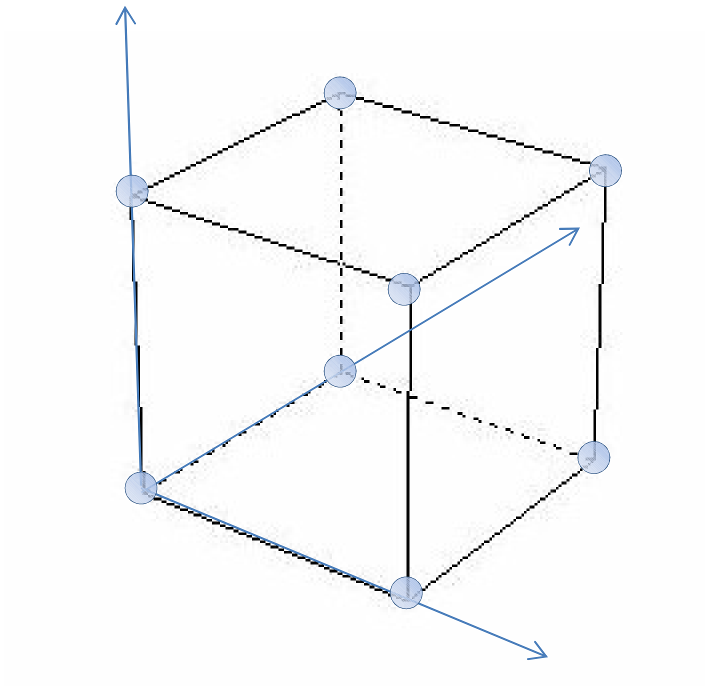
- Problem: Network may just learn the values at the inputs
  - Learn the red curve instead of the dotted blue one
    - Given only the red vertical bars as inputs

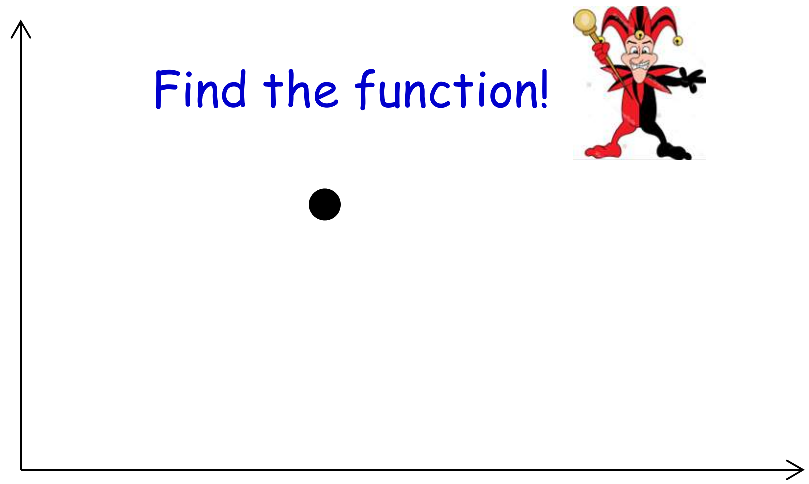
Data under-specification



- Consider a binary 100-dimensional input
- There are $2^{100}=10^{30}$ possible inputs
- Complete specification of the function will require specification of 10^{30} output values
- A training set with only 10^{15} training instances will be off by a factor of 10^{15}

Data under-specification in learning





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- There are $2^{100}=10^{30}$ possible inputs
- Complete specification of the function will require specification of 10^{30} output values
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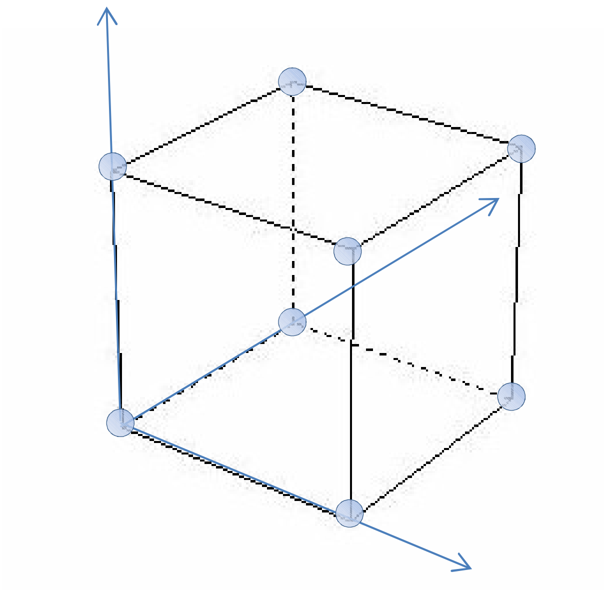
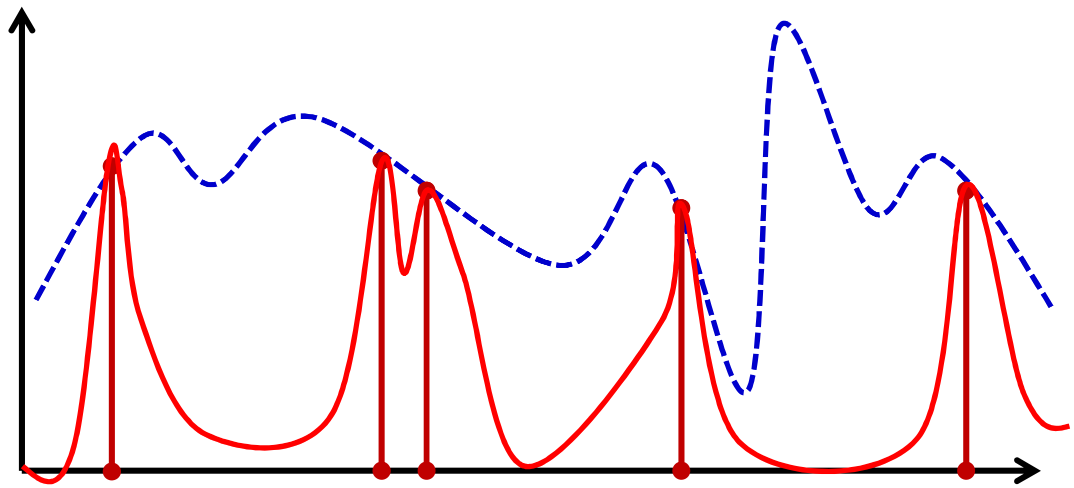
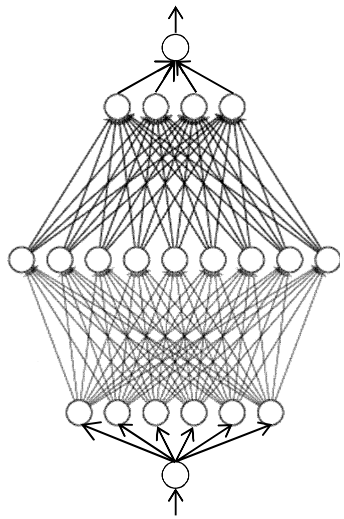
Need “smoothing” constraints

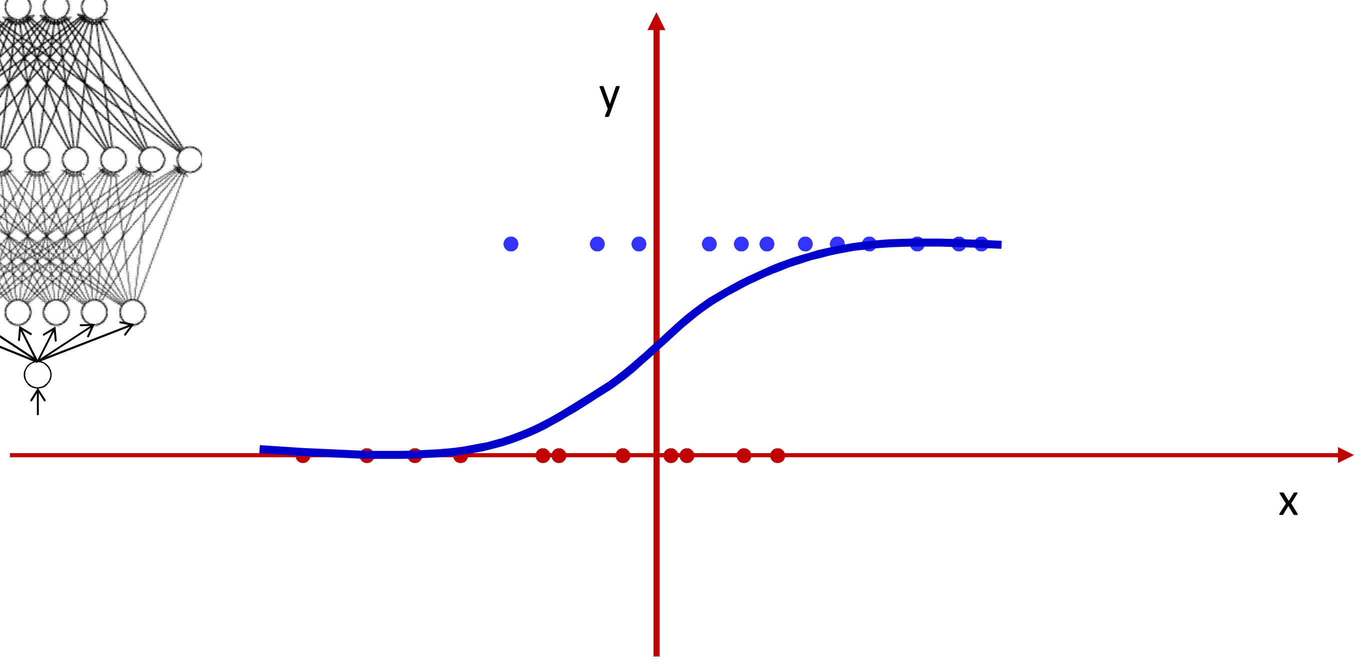




- Need additional constraints that will “fill in” the missing regions acceptably
  - Generalization

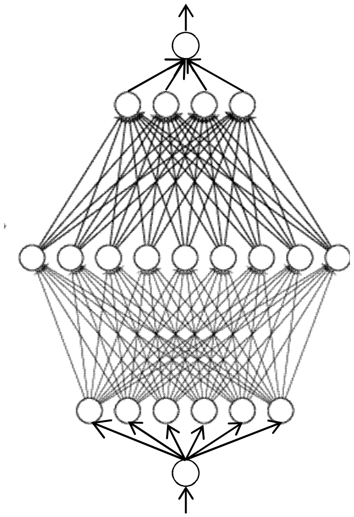
Smoothness through weight manipulation

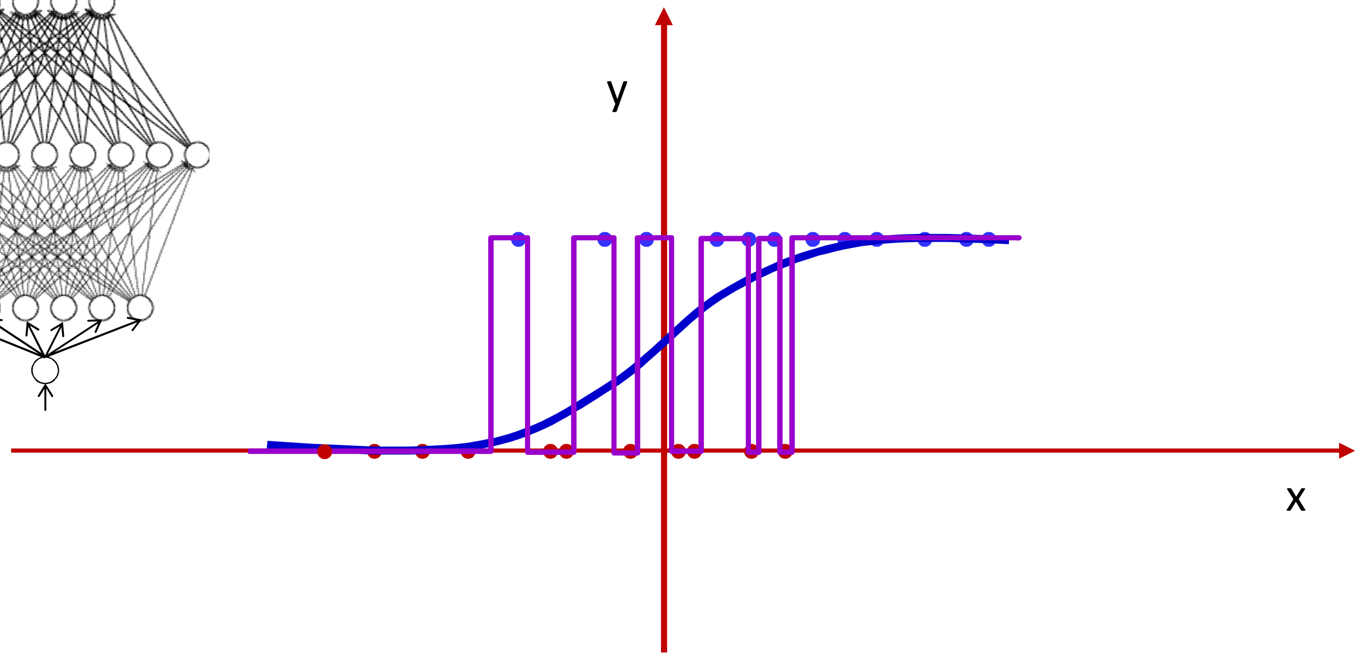




- Illustrative example: Simple binary classifier
  – The “desired” output is generally smooth

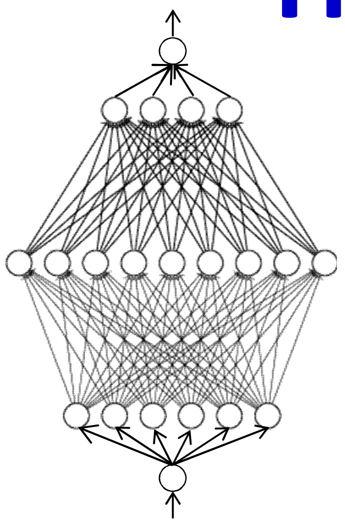
Smoothness through weight manipulation

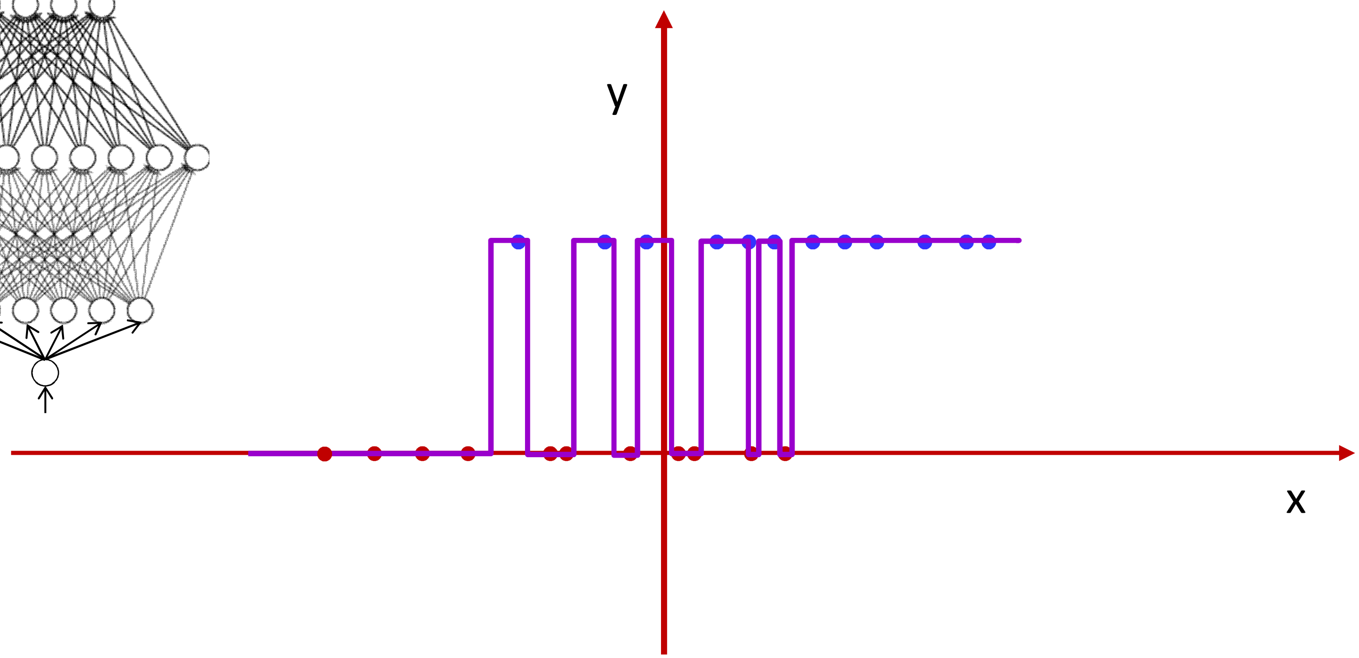




- Illustrative example: Simple binary classifier
  - The “desired” output is generally smooth
    - Capture statistical or average trends
  - An unconstrained model will model individual instances instead

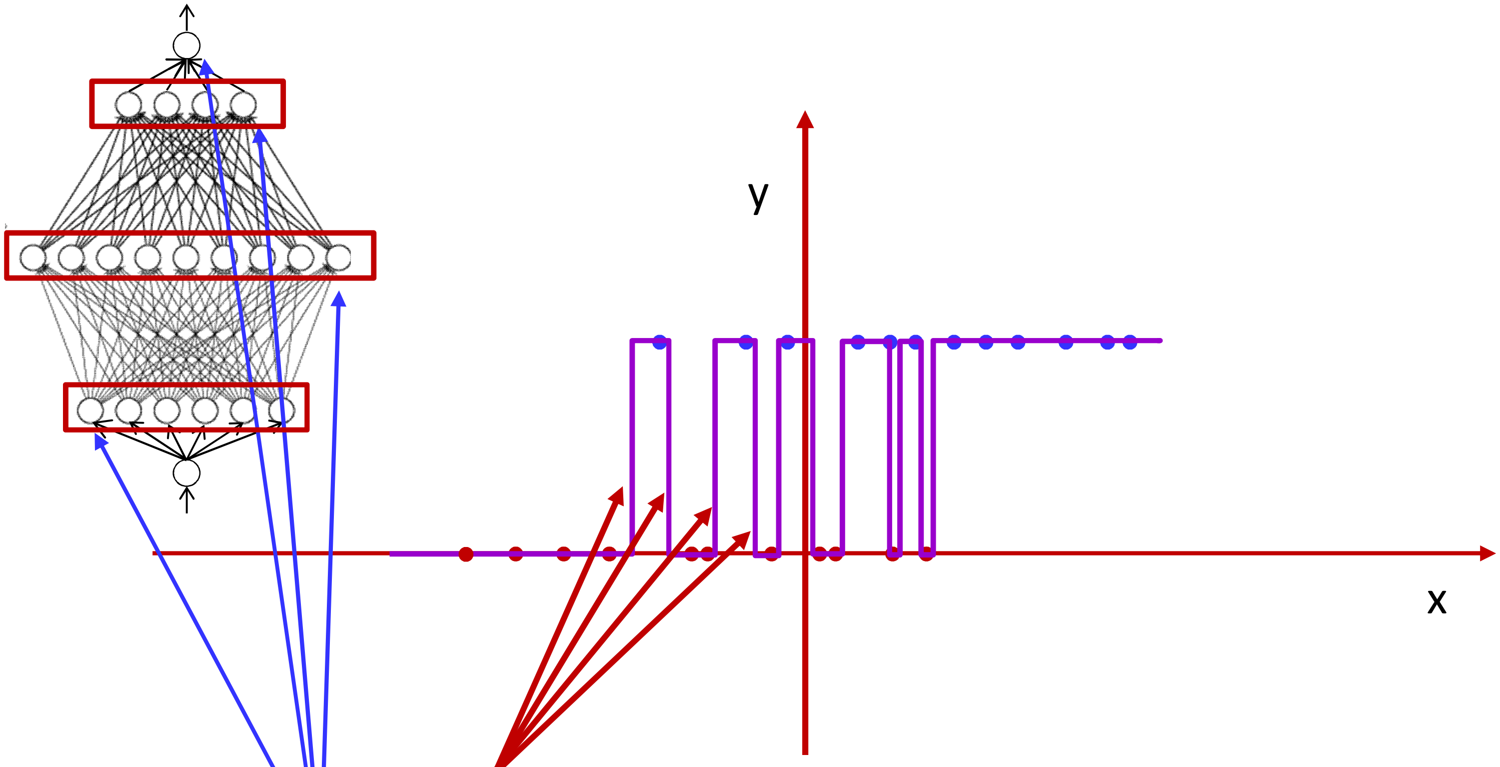
The unconstrained model





- Illustrative example: Simple binary classifier
  - The "desired" output is generally smooth
    - Capture statistical or average trends
  - An unconstrained model will model individual instances instead

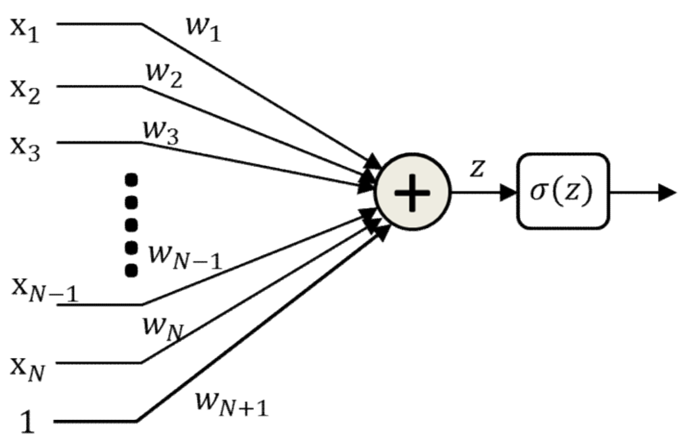
Why overfitting

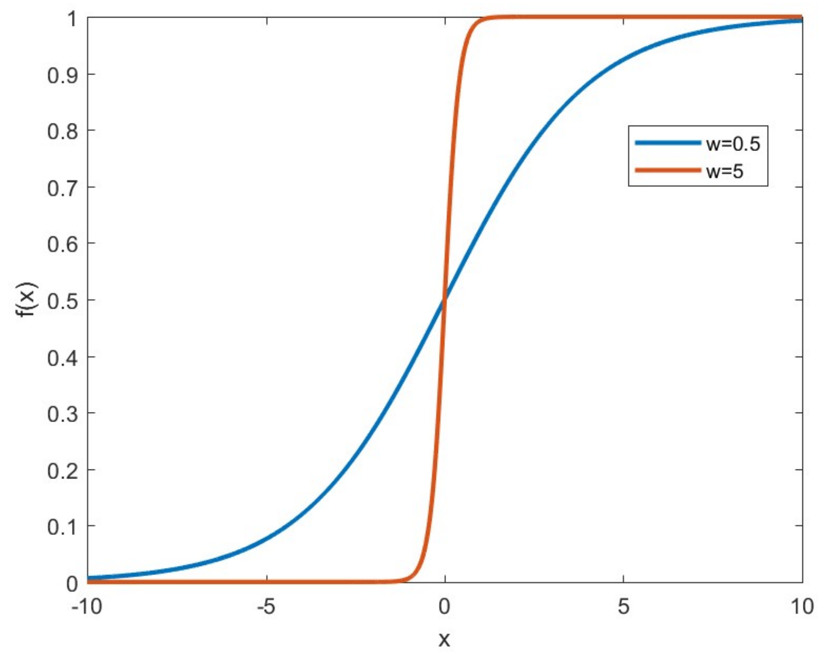


These sharp changes happen because ..

..the perceptrons in the network are individually capable of sharp changes in output

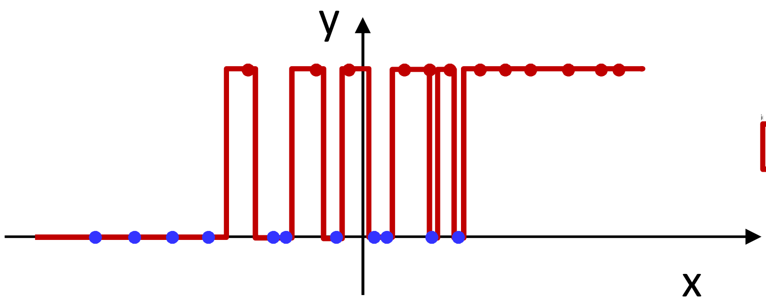
The individual perceptron

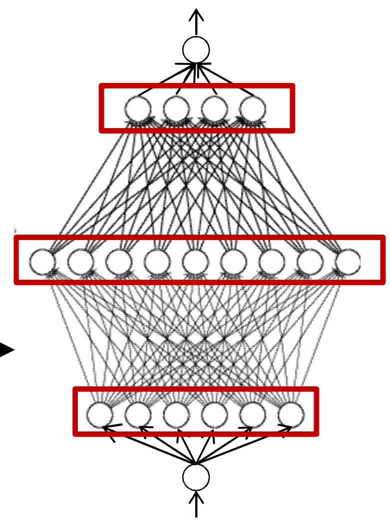


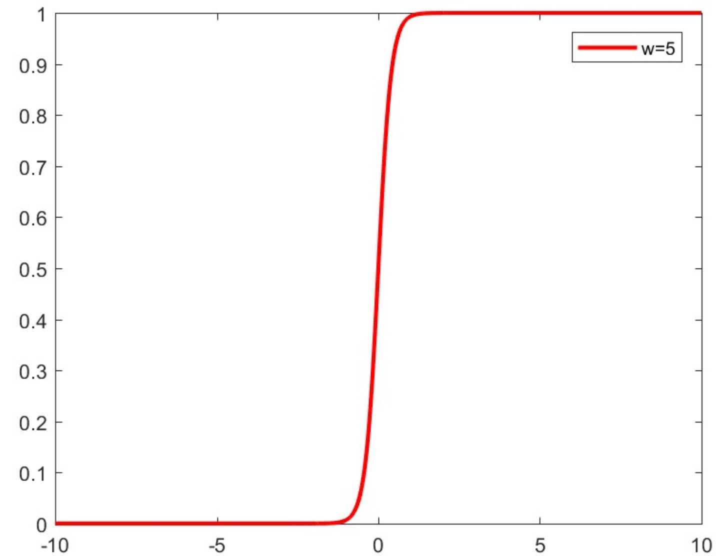


- Using a sigmoid activation
  - As $|w|$ increases, the response becomes steeper

Smoothness through weight manipulation

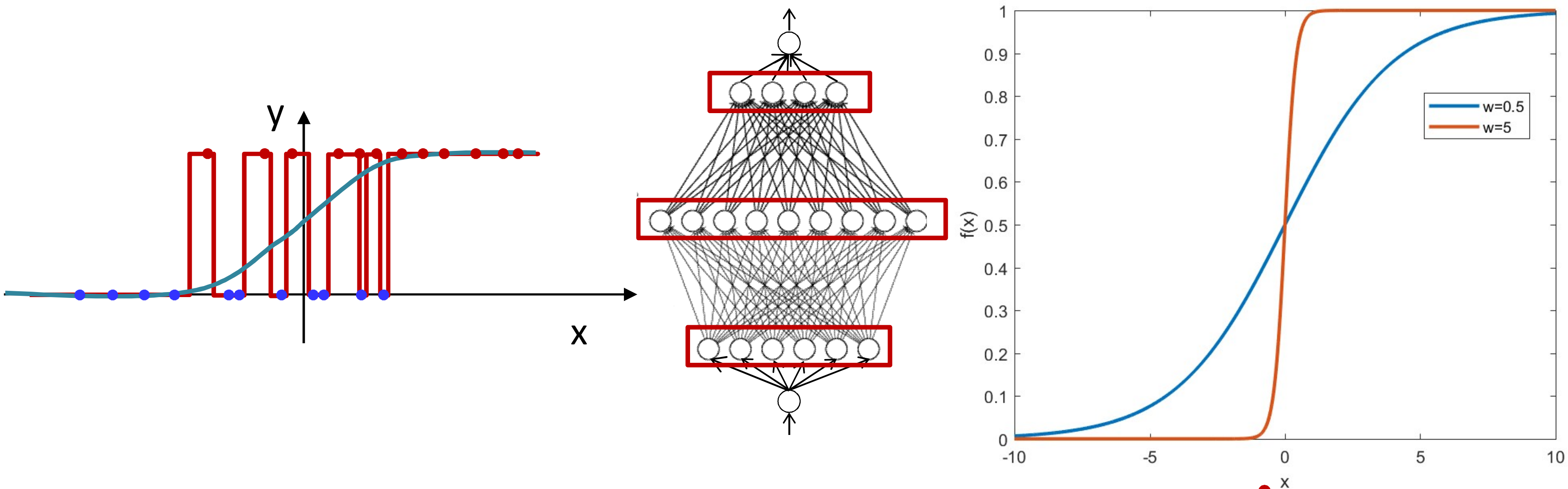






- Steep changes that enable overfitted responses are facilitated by perceptrons with large *w*

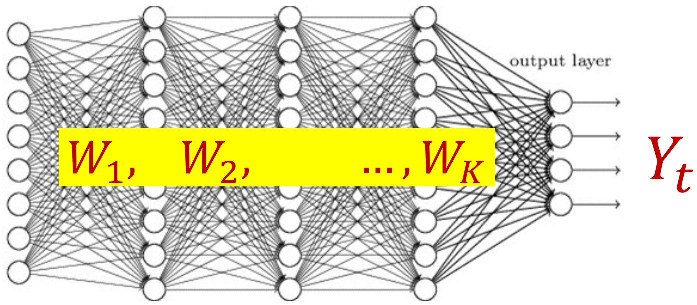
Smoothness through weight manipulation



- Steep changes that enable overfitted responses are facilitated by perceptrons with large *w*

- Constraining the weights *w* to be low will force slower perceptrons and smoother output response

Objective function for neural networks



Desired output of network: d_t

Error on i-th training input: $Div(Y_t, d_t; W_1, W_2, \ldots, W_K)$

Batch training loss:

$$Loss(W_1, W_2, \ldots, W_K) = \frac{1}{T} \sum_t Div(Y_t, d_t; W_1, W_2, \ldots, W_K)$$

- Conventional training: minimize the total loss:

$$\widehat{W}_1, \widehat{W}_2, \ldots, \widehat{W}_K = \underset{W_1, W_2, \ldots, W_K}{\operatorname{argmin}} Loss(W_1, W_2, \ldots, W_K)$$

Smoothness through weight constraints

- Regularized training: minimize the loss while also minimizing the weights

$$L(W_1, W_2, \ldots, W_K) = Loss(W_1, W_2, \ldots, W_K) + \frac{1}{2}\lambda \sum_k \|W_k\|_2^2$$

$$\widehat{W}_1, \widehat{W}_2, \ldots, \widehat{W}_K = \underset{W_1, W_2, \ldots, W_K}{\operatorname{argmin}} \; L(W_1, W_2, \ldots, W_K)$$

- λ is the regularization parameter whose value depends on how important it is for us to want to minimize the weights

- Increasing λ assigns greater importance to shrinking the weights
  - Make greater error on training data, to obtain a more acceptable network

Regularizing the weights

$$L(W_1, W_2, \dots, W_K) = \frac{1}{T}\sum_t Div(Y_t, d_t) + \frac{1}{2}\lambda \sum_k \|W_k\|_2^2$$

- Batch mode:

$$\Delta W_k = \frac{1}{T}\sum_t \nabla_{W_k} Div(Y_t, d_t)^T + \lambda W_k$$

- SGD:

$$\Delta W_k = \nabla_{W_k} Div(Y_t, d_t)^T + \lambda W_k$$

- Minibatch:

$$\Delta W_k = \frac{1}{b}\sum_{\tau=t}^{t+b-1} \nabla_{W_k} Div(Y_\tau, d_\tau)^T + \lambda W_k$$

- Update rule:

$$W_k \leftarrow W_k - \eta \Delta W_k$$

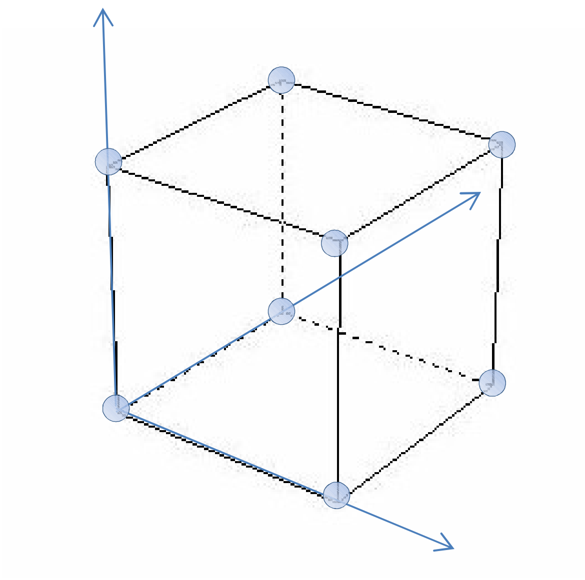
Incremental Update: Mini-batch update

- 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 $\nabla_{W_k} Div(Y_t, d_t)$
        - » $\Delta W_k = \Delta W_k + \nabla_{W_k} Div(Y_t, d_t)^T$
    - Update
      - For every layer k:

$$W_k = W_k - \eta_j(\Delta W_k + \lambda W_k)$$

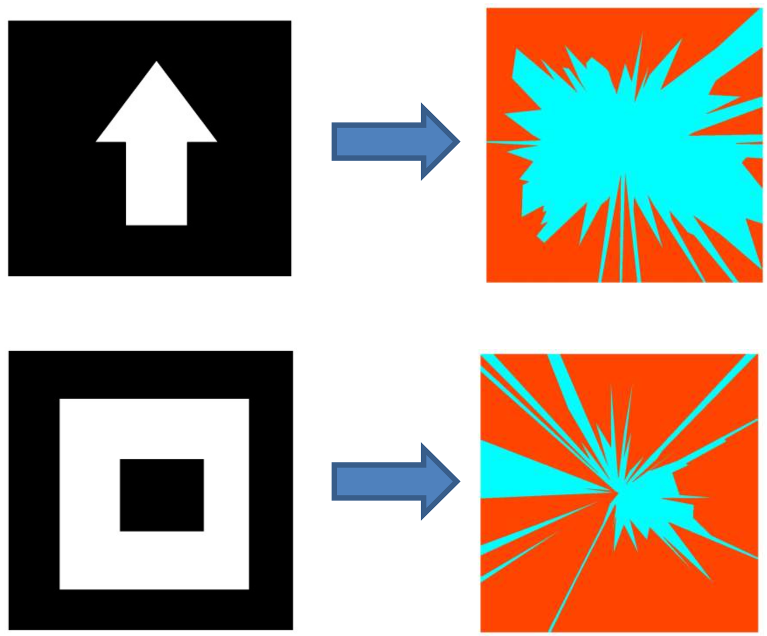
- Until Err has converged

Smoothness through network structure



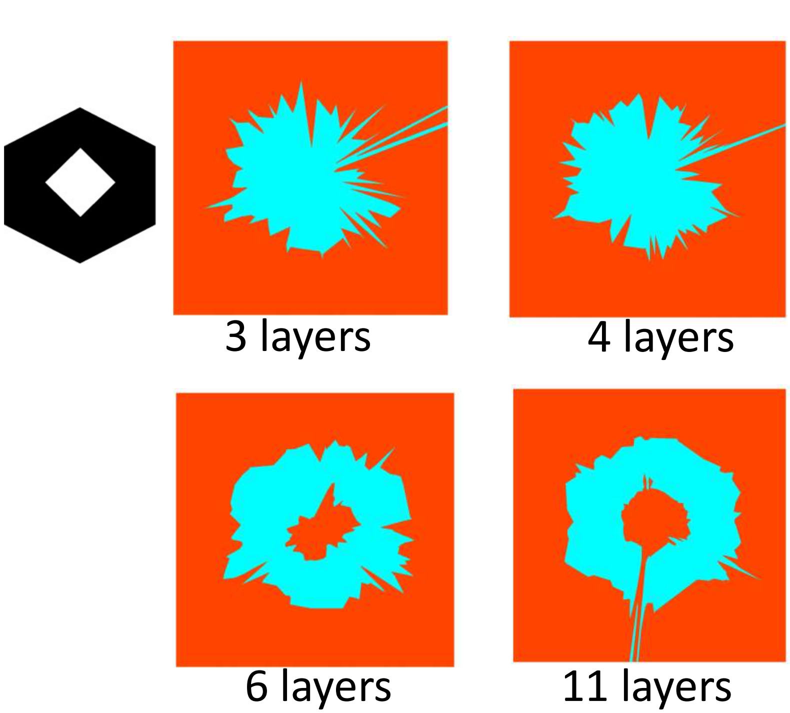
- MLPs naturally impose constraints
- MLPs are universal approximators
  - Arbitrarily increasing size can give you arbitrarily wiggly functions
  - The function will remain ill-defined on the majority of the space
- *For a given number of parameters deeper networks impose more smoothness than shallow ones*
  - Each layer works on the already smooth surface output by the previous layer

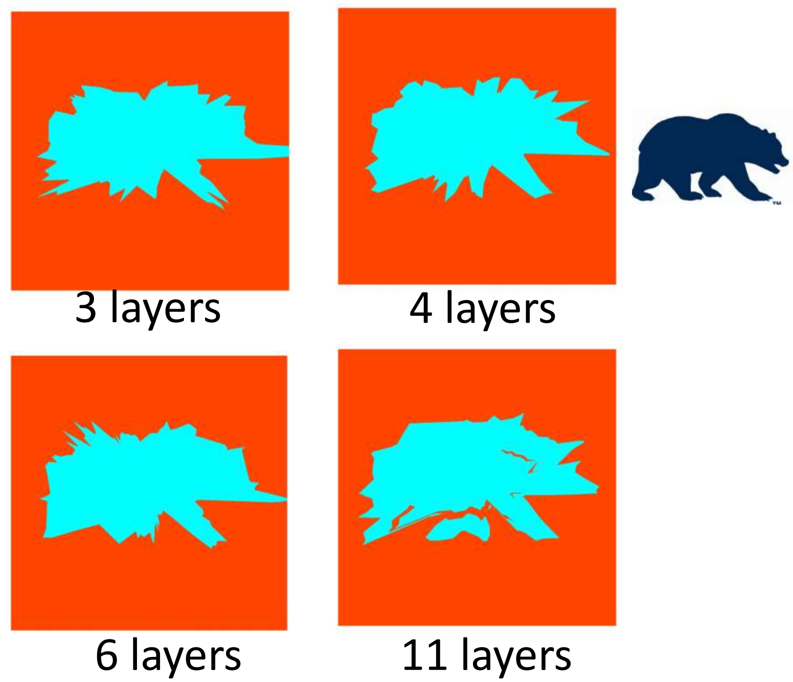
Even when we get it all right



- Typical results (varies with initialization)
- 1000 training points – orders of magnitude more than you usually get
- All the training tricks known to mankind

But depth and training data help





- Deeper networks seem to learn better, for the same number of total neurons
  - ***Implicit smoothness constraints***
    - ***As opposed to explicit constraints from more conventional classification models***

- **Similar functions not learnable using more usual pattern-recognition models!!**

10000 training instances

Regularization..

- Other techniques have been proposed to improve the smoothness of the learned function
  - L_1 regularization of network activations
  - Regularizing with added noise..

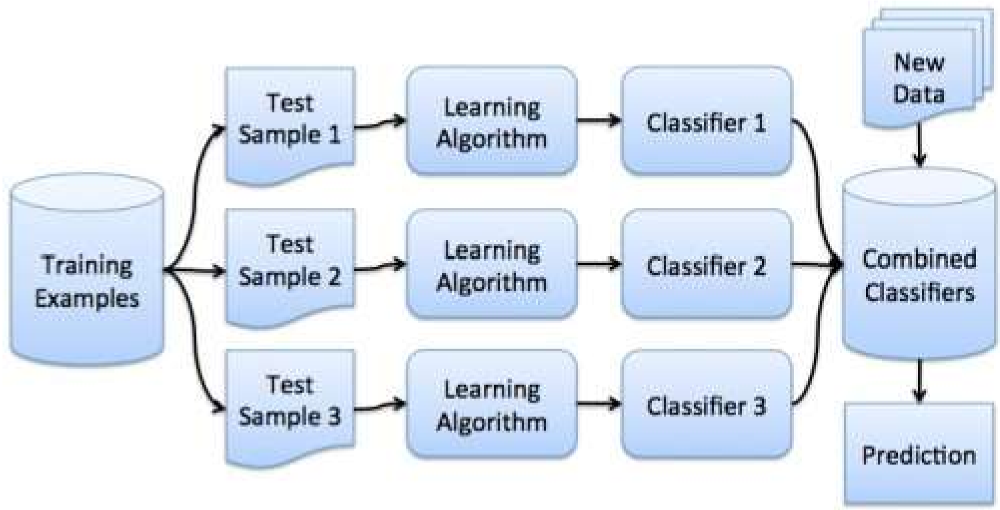
- Possibly the most influential method has been "dropout"

Story so far

- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

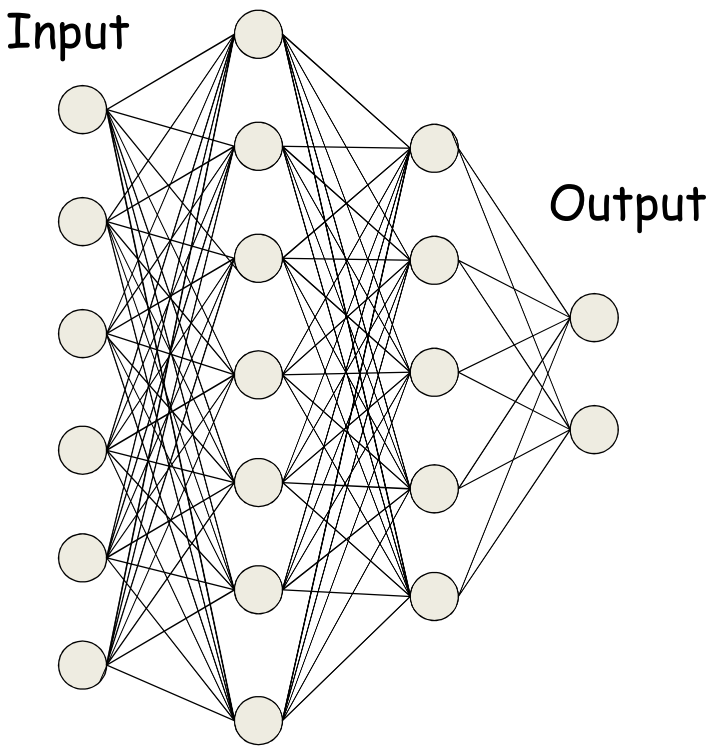
- The choice of divergence affects both the learned network and results
- Covariate shift between training and test may cause problems and may be handled by batch normalization
- Data underspecification can result in overfitted models and must be handled by regularization and more constrained (generally deeper) network architectures

A brief detour.. Bagging



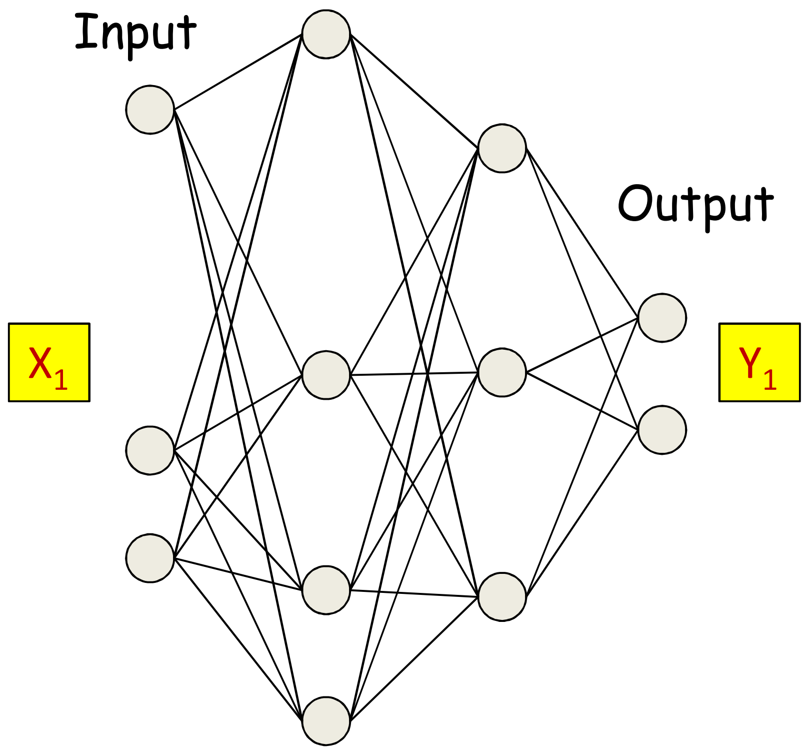
- Popular method proposed by Leo Breiman:
  - Sample training data and train several different classifiers
  - Classify test instance with entire ensemble of classifiers
  - Vote across classifiers for final decision
  - Empirically shown to improve significantly over training a single classifier from combined data
- Returning to our problem....

Dropout



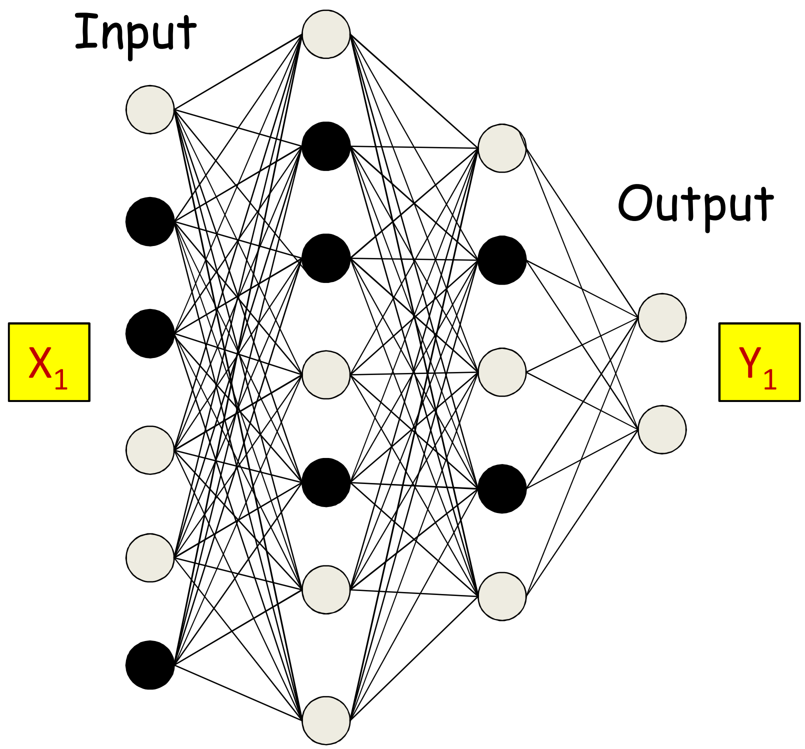
- **During training:** For each input, at each iteration, "turn off" each neuron with a probability 1-α

Dropout



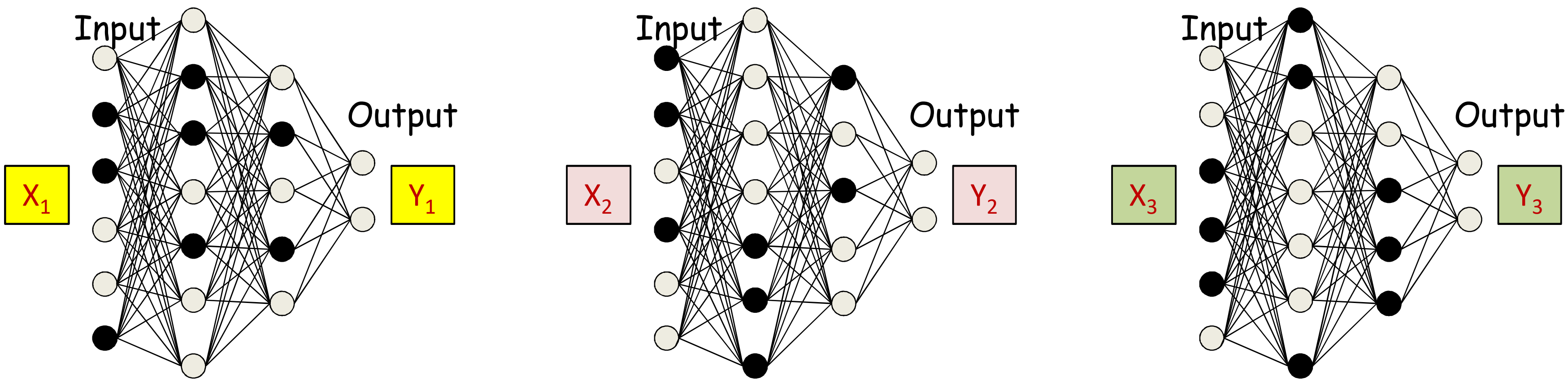
- **During training:** For each input, at each iteration, "turn off" each neuron with a probability 1-α
  - Also turn off inputs similarly

Dropout



- **During training:** For each input, at each iteration, "turn off" each neuron (including inputs) with a probability $1-\alpha$
  - In practice, set them to 0 according to the success of a Bernoulli random number generator with success probability $1-\alpha$

Dropout



The pattern of dropped nodes changes for *each input*
i.e. in every pass through the net

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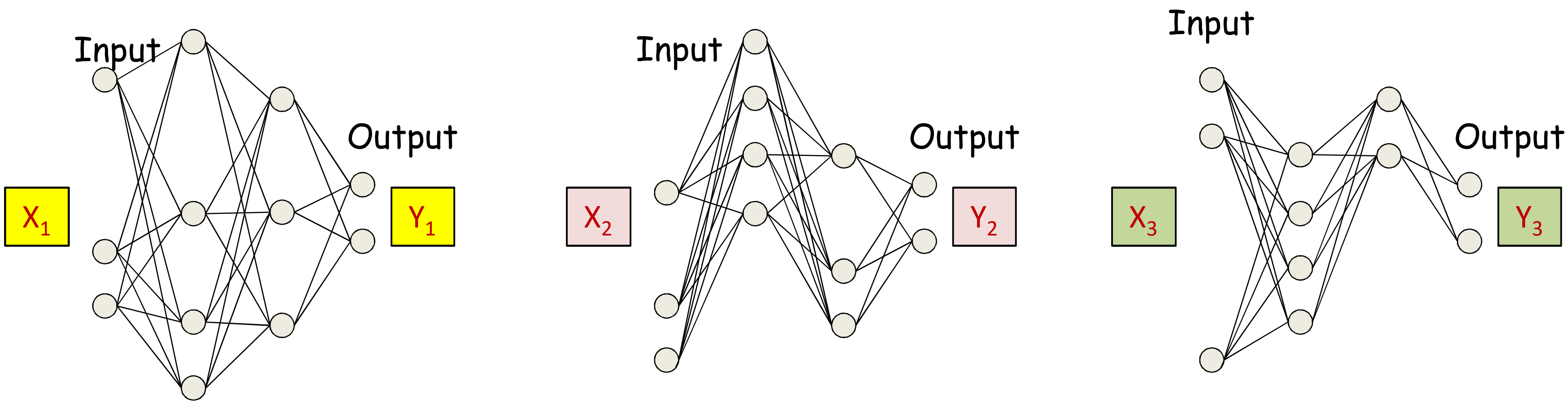
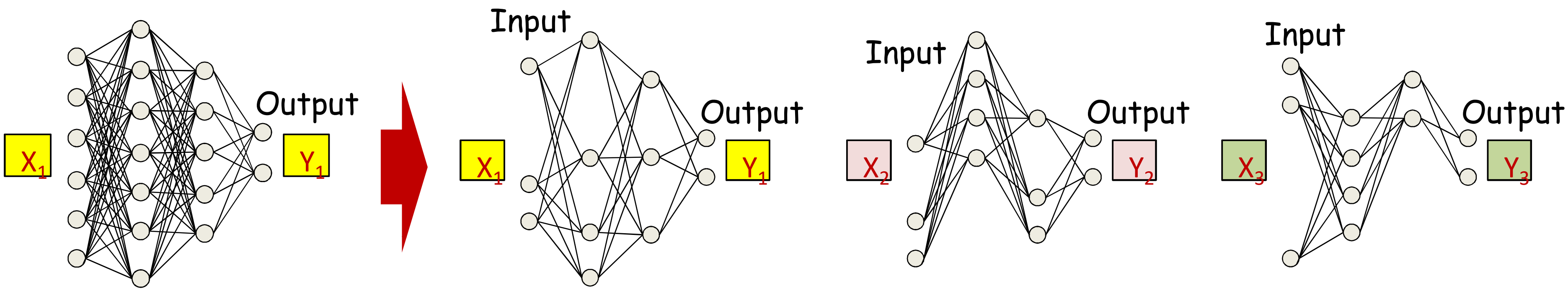
Dropout



The pattern of dropped nodes
changes for *each input*
i.e. in every pass through the net

- **During training:** Backpropagation is effectively performed only over the remaining network
  - The effective network is different for different inputs
  - Gradients are obtained only for the weights and biases *from* "On" nodes *to* "On" nodes
    - For the remaining, the gradient is just 0

Statistical Interpretation



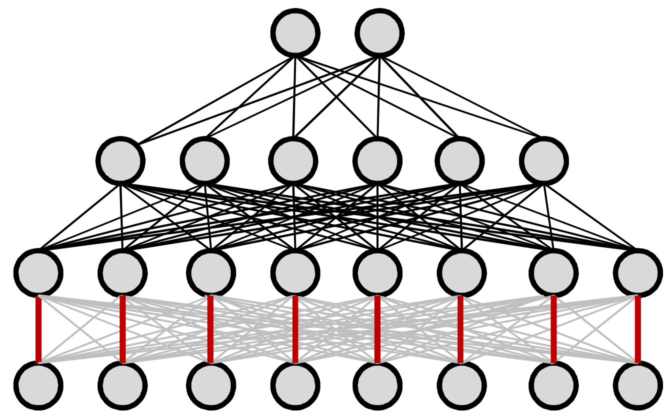
- For a network with a total of N neurons, there are 2^N possible sub-networks
  - Obtained by choosing different subsets of nodes
  - Dropout *samples* over all 2^N possible networks
  - Effectively learns a network that *averages* over all possible networks
    - Bagging

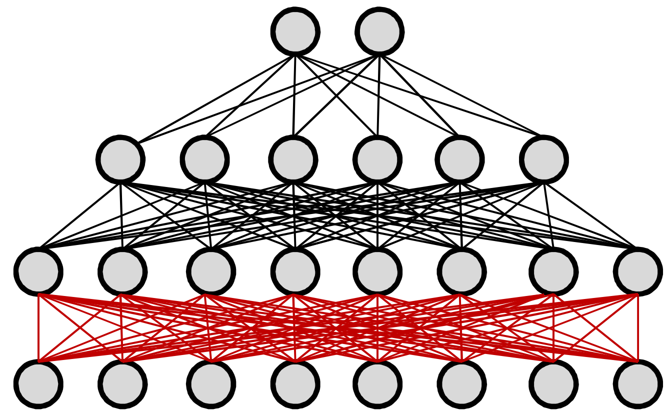
Dropout as a mechanism to increase pattern density

- Dropout forces the neurons to learn "rich" and redundant patterns

- E.g. without dropout, a non-compressive layer may just "clone" its input to its output
  - Transferring the task of learning to the rest of the network upstream

- Dropout forces the neurons to learn denser patterns
  - With redundancy





The forward pass

- Input: D dimensional vector $\mathbf{x} = [x_j,\ j = 1 \dots D]$
- Set:
  - $D_0 = D,$ is the width of the 0th (input) layer
  - $y_j^{(0)} = x_j,\ j = 1 \dots D; \qquad y_0^{(k=1\dots N)} = x_0 = 1$
- For layer $k = 1 \dots N$
  - For $j = 1 \dots D_k$
    - $z_j^{(k)} = \sum_{i=0}^{N_k} w_{i,j}^{(k)} y_i^{(k-1)} + b_j^{(k)}$
    - $y_j^{(k)} = f_k\left(z_j^{(k)}\right)$
    - If $(k\ =\ dropout\ layer):$
      - $mask(k,j) =\ Bernoulli(\alpha)$
      - If $mask(k,j) == 0$
        - » $y_j^{(k)} = 0$
- Output:
  - $Y = y_j^{(N)}, j = 1..D_N$

Backward Pass

- Output layer (N) :
  - $\frac{\partial Div}{\partial Y_i} = \frac{\partial Div(Y,d)}{\partial y_i^{(N)}}$
  - $\frac{\partial Div}{\partial z_i^{(k)}} = f_k'\left(z_i^{(k)}\right)\frac{\partial Div}{\partial y_i^{(k)}}$
- For layer $k = N - 1\ downto\ 0$
  - For $i = 1 \dots D_k$
    - If (not dropout layer OR $mask(k,i)$)
      - $\frac{\partial Div}{\partial y_i^{(k)}} = \sum_j w_{ij}^{(k+1)} \frac{\partial Div}{\partial z_j^{(k+1)}} mask(k+1,j)$
      - $\frac{\partial Div}{\partial z_i^{(k)}} = f_k'\left(z_i^{(k)}\right)\frac{\partial Div}{\partial y_i^{(k)}}$
      - $\frac{\partial Div}{\partial w_{ij}^{(k+1)}} = y_i^{(k)} \frac{\partial Div}{\partial z_j^{(k+1)}} mask(k+1,j)$ for $j = 1 \dots D_{k+1}$
    - Else
      - $\frac{\partial Di}{\partial z_i^{(k)}} = 0$

What each neuron computes

- Each neuron actually has the following activation:

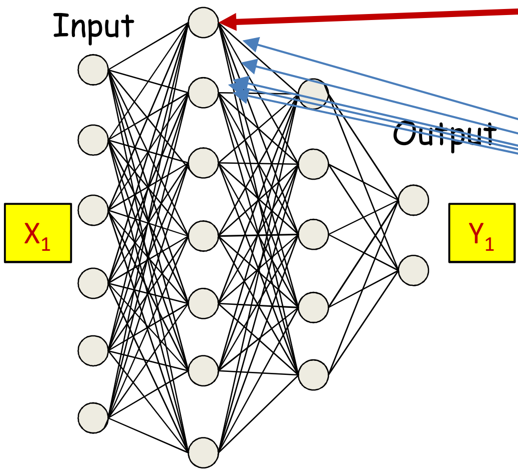
$$y_i^{(k)} = D\sigma\left(\sum_j w_{ji}^{(k)} y_j^{(k-1)} + b_i^{(k)}\right)$$

  - Where D is a Bernoulli variable that takes a value 1 with probability α
- D may be switched on or off for individual sub networks, but over the ensemble, the *expected output* of the neuron is

$$y_i^{(k)} = \alpha\sigma\left(\sum_j w_{ji}^{(k)} y_j^{(k-1)} + b_i^{(k)}\right)$$

- During *test* time, we will use the *expected* output of the neuron
  - Which corresponds to the bagged average output
  - Consists of simply scaling the output of each neuron by α

Dropout during test: implementation



apply α here (to the output of the neuron) OR..

Push the α to all outgoing weights

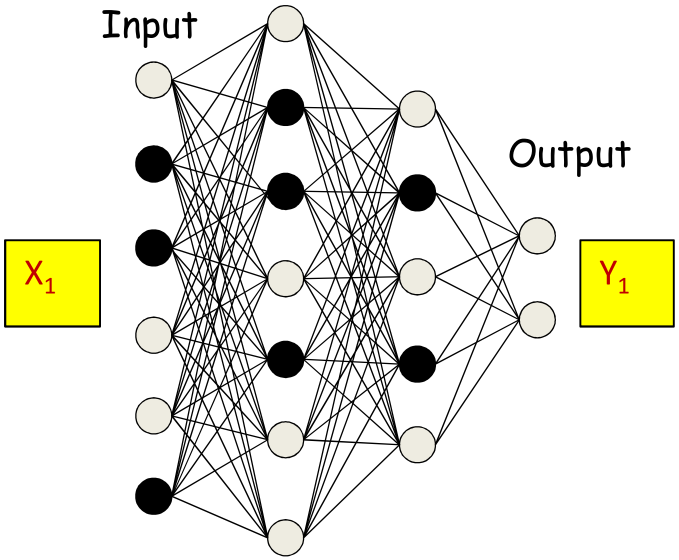
$$\boldsymbol{y_i^{(k)}} = \alpha\boldsymbol{\sigma}\left(\boldsymbol{z_i^{(k)}}\right)$$

$$\begin{aligned} z_i^{(k)} &= \sum_j w_{ji}^{(k)} y_j^{(k-1)} + b_i^{(k)} \\ &= \sum_j w_{ji}^{(k)} \alpha\sigma\left(z_j^{(k-1)}\right) + b_i^{(k)} \\ &= \sum_j \left(\alpha w_{ji}^{(k)}\right)\sigma\left(z_j^{(k-1)}\right) + b_i^{(k)} \end{aligned}$$

$$W_{test} = \alpha W_{trained}$$

- Instead of multiplying every output by α, multiply all weights by α

Dropout : alternate implementation

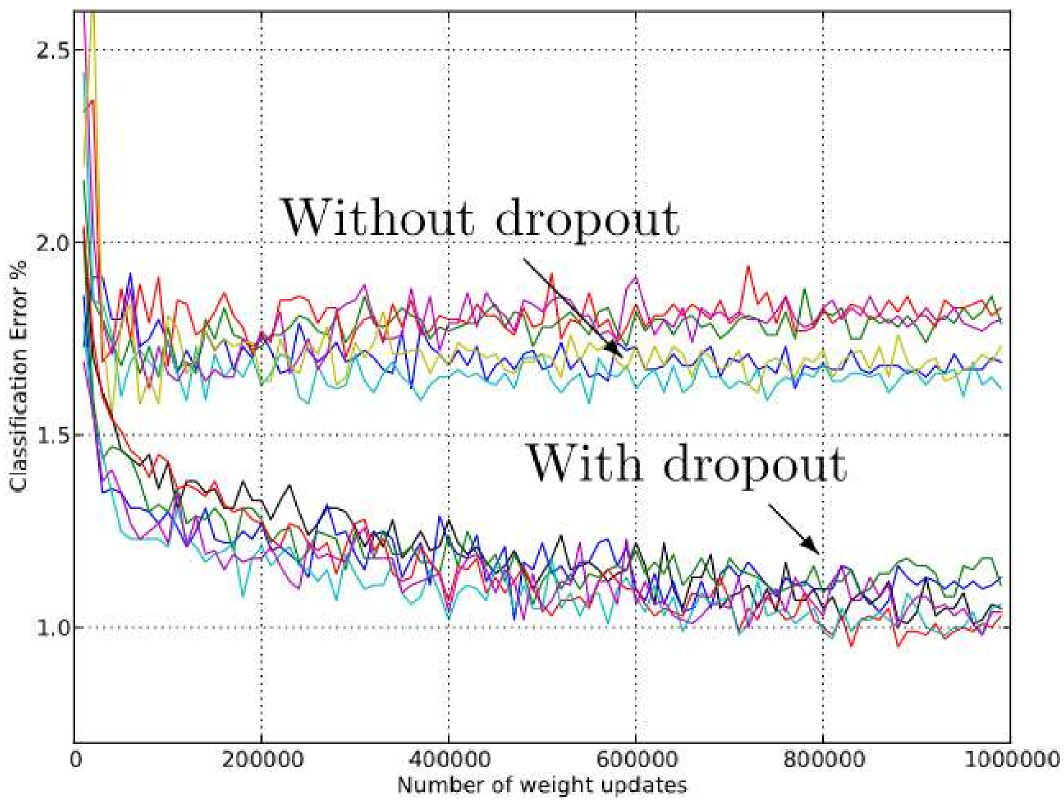


- Alternately, during *training,* replace the activation of all neurons in the network by $\alpha^{-1}\sigma(.)$
  - This does not affect the dropout procedure itself
  - We will use $\sigma(.)$ as the activation during testing, and not modify the weights

The forward pass (testing)

- Input: D dimensional vector $\mathbf{x} = [x_j,\ j = 1 \dots D]$
- Set:
  - $D_0 = D,$ is the width of the 0th (input) layer
  - $y_j^{(0)} = x_j,\ j = 1 \dots D; \quad y_0^{(k=1 \dots N)} = x_0 = 1$
- For layer $k = 1 \dots N$
  - For $j = 1 \dots D_k$
    - $z_j^{(k)} = \sum_{i=0}^{N_k} w_{i,j}^{(k)} y_i^{(k-1)} + b_j^{(k)}$
    - $y_j^{(k)} = f_k\left(z_j^{(k)}\right)$
    - If $(k = dropout\ layer)$:
      - » $y_j^{(k)} = y_j^{(k)}/\alpha$
    - Else
      - » $y_j^{(k)} = 0$
- Output:
  - $Y = y_j^{(N)}, j = 1..D_N$

Dropout: Typical results



- From Srivastava et al., 2013. Test error for different architectures on MNIST with and without dropout
  - 2-4 hidden layers with 1024-2048 units

Variations on dropout

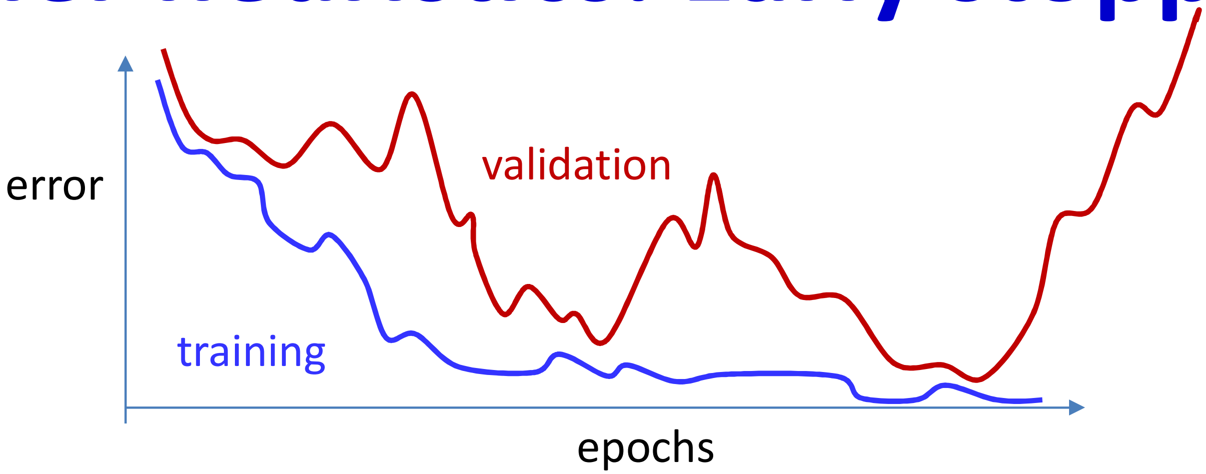
- Zoneout: For RNNs
  - Randomly chosen units remain unchanged across a time transition
- Dropconnect
  - Drop individual connections, instead of nodes
- Shakeout
  - Scale *up* the weights of randomly selected weights
    - $|w| \rightarrow \alpha|w| + (1 - \alpha)c$
  - Fix remaining weights to a negative constant
    - $w \rightarrow -c$
- Whiteout
  - Add or multiply weight-dependent Gaussian noise to the signal on each connection

Story so far

- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

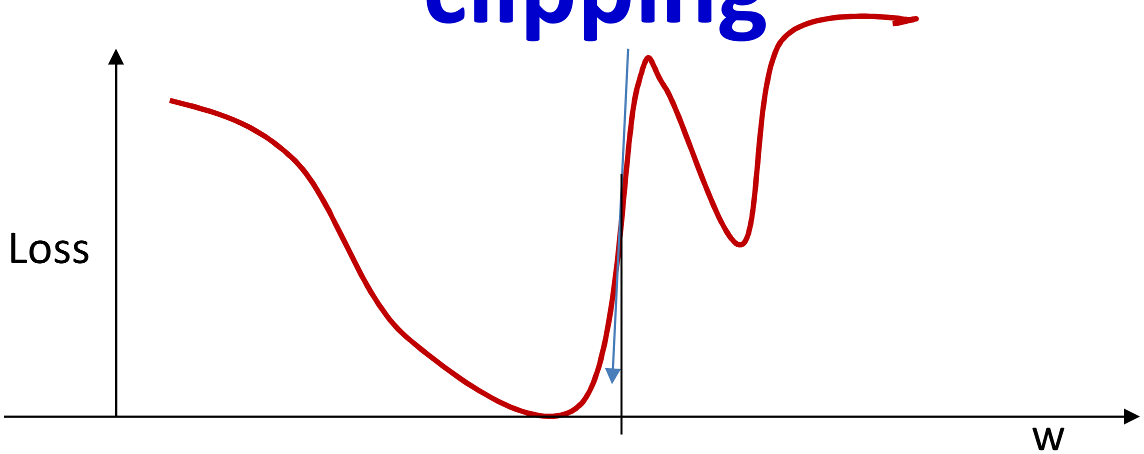
- The choice of divergence affects both the learned network and results
- Covariate shift between training and test may cause problems and may be handled by batch normalization
- Data underspecification can result in overfitted models and must be handled by regularization and more constrained (generally deeper) network architectures
- "Dropout" is a stochastic data/model erasure method that sometimes forces the network to learn more robust models

Other heuristics: Early stopping



- Continued training can result in over fitting to training data
  - Track performance on a held-out validation set
  - Apply one of several early-stopping criterion to terminate training when performance on validation set degrades significantly

Additional heuristics: Gradient clipping

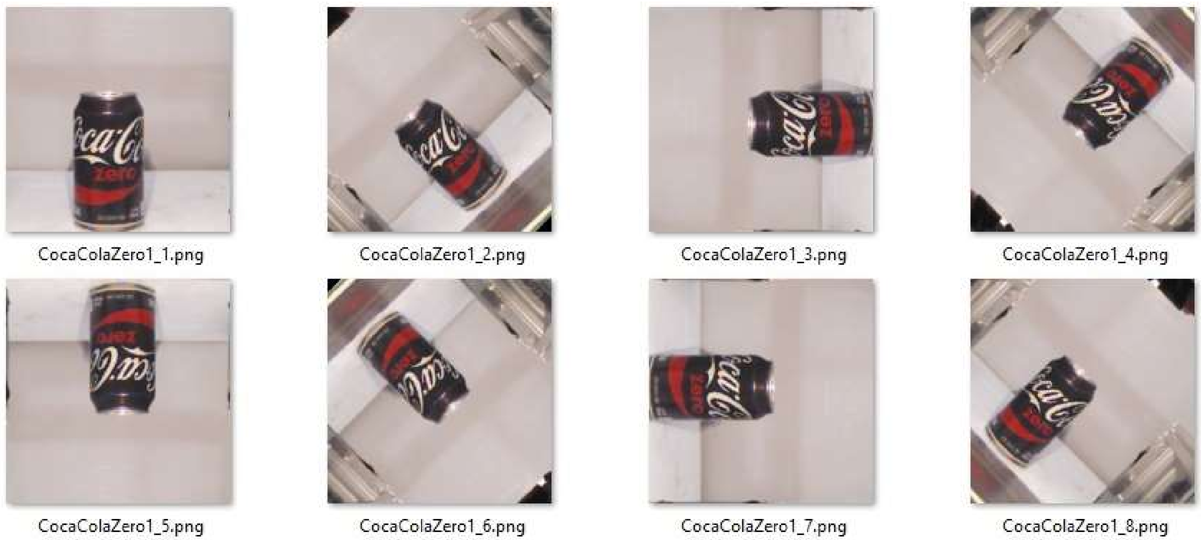


- Often the derivative will be too high
  - When the divergence has a steep slope
  - This can result in instability
- **Gradient clipping**: set a ceiling on derivative value

$$if\ \partial_w D > \theta\ then\ \partial_w D = \theta$$

  - Typical θ value is 5

Additional heuristics: Data Augmentation



- Available training data will often be small
- "Extend" it by distorting examples in a variety of ways to generate synthetic labelled examples
  - E.g. rotation, stretching, adding noise, other distortion

Other tricks

- Normalize the input:
  - Apply covariate shift to entire training data to make it 0 mean, unit variance
  - Equivalent of batch norm on input
- A variety of other tricks are applied
  - Initialization techniques
    - Typically initialized randomly
    - Key point: neurons with identical connections that are identically initialized will never diverge
  - Practice makes man perfect

Setting up a problem

- Obtain training data
  - Use appropriate representation for inputs and outputs
- Choose network architecture
  - More neurons need more data
  - Deep is better, but harder to train
- Choose the appropriate divergence function
  - Choose regularization
- Choose heuristics (batch norm, dropout, etc.)
- Choose optimization algorithm
  - E.g. Adagrad
- Perform a grid search for hyper parameters (learning rate, regularization parameter, …) on held-out data
- Train
  - Evaluate periodically on validation data, for early stopping if required

In closing

- Have outlined the process of training neural networks
  - Some history
  - A variety of algorithms
  - Gradient-descent based techniques
  - Regularization for generalization
  - Algorithms for convergence
  - Heuristics
- Practice makes perfect..