Deep Learning (BEV033DLE)
Lecture 4. SGD

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✦ Definitions and Main Properties

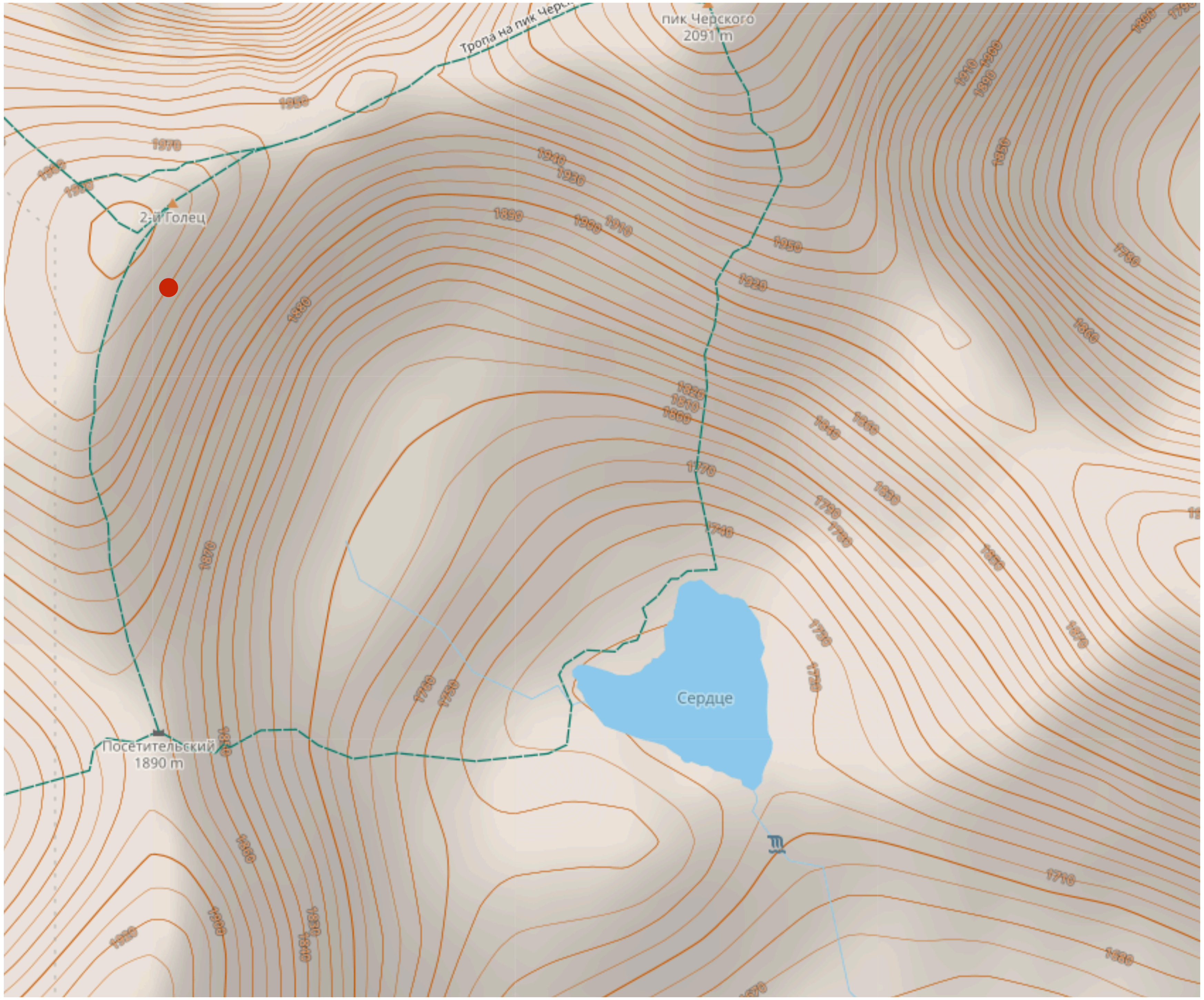
- Gradient Descent and SGD
- Convergence properties, step size

✦ Important Details

- Dataset sampling with and without replacement
- How to monitor progress, Running averages
- Momentum
- Implicit regularization: early stopping, batch size and weight norm

Stochastic Gradient Descent

$L(\theta)$



- Gradient Descent:
  - $g_t = \nabla_\theta L(\theta_t)$
  - $\theta_{t+1} = \theta_t - \alpha_t g_t$

- SGD:
  - Noisy gradient $\tilde{g}_t$
  - $\mathbb{E}[\tilde{g}_t] = g_t$
  - $\theta_{t+1} = \theta_t - \alpha_t \tilde{g}_t$

SGD for Statistical Estimation

- Problem Setup:
  - Training set: $\mathcal{T} = (x_i, y_i)_{i=1}^n$ – i.i.d.
  - Predictor: $f(x; \theta)$, θ – vector of all parameters θ
  - Negative log-likelihood: $L = \frac{1}{n}\sum_i l(y_i, f(x_i; \theta)) = \frac{1}{n}\sum_i l_i(\theta)$
  - Learning problem: $\min\limits_{\theta} L(\theta)$

- Examples
  - Regression in $\mathbb{R}^m$:

    $f(x; \theta) \in \mathbb{R}^m$ – predicted values

    Squared error loss: $l_i = \|y_i - f(x_i; \theta)\|^2$
  - Classification with K classes:

    $f(x) \in \mathbb{R}^K$ – scores

    Predictive probabilities $p(y = k|x) = \mathrm{softmax}(f(x; \theta))_k$

    NLL loss: $l_i(\theta) = -(\log \mathrm{softmax}(f(x_i; \theta)))_{y_i}$

SGD for Statistical Estimation

- Gradient Descent (**GD**):
  - Gradient at current point θ_t: $g_t = \nabla L(\theta_t) = \frac{1}{n}\sum_i \nabla l_i(\theta_t)$
  - Make a small step in the steepest descent direction of L:
  - $\theta_{t+1} = \theta_t - \alpha_t g_t$
  - Historically called "'batch gradient descent"
  - If the dataset is very large, lots of computation to make a small step

- Stochastic Gradient Descent (**SGD**):
  - Pick M data points $I = \{i_1, \ldots i_M\}$ at random
  - Estimate gradient as $\tilde{g}_t = \frac{1}{M}\sum_{i\in I} \nabla l_i(\theta_t)$
  - $\theta_{t+1} = \theta_t - \alpha_t \tilde{g}_t$
  - $\{(x_i, y_i) \,|\, i \in I\}$ is called a **(mini)-batch**

- "Noisy" gradient $\tilde{g}_t$:
  - $\mathbb{E}[\tilde{g}_t] = g_t$
  - $\mathbb{V}[\tilde{g}_t] = \frac{1}{M}\mathbb{V}[\tilde{g}_t^1]$, where $\tilde{g}^1$ is stochastic gradient with 1 sample
  - Diminishing gain in accuracy with larger batch size M
  - In the beginning a small subset of data suffices for a good direction

More General Form

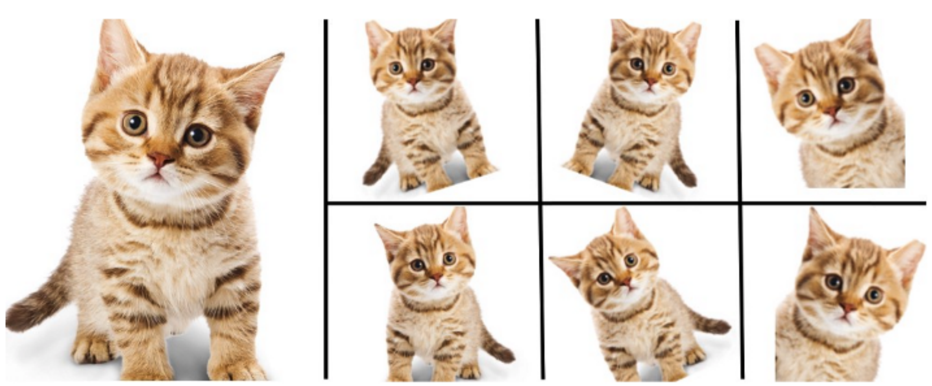
- SGD in Machine learning:
  - Specialized loss functions (not necessary likelihood), additive in training data
  - Training set possibly infinite (augmentation)

- Problem Setup:
  - Loss: $L(\theta) = \mathbb{E}_{(x,y)\sim p^*}[l(y, f(x;\theta))] + R(\theta)$
  - Training set is given as a generator p^*
  - $R(\theta)$ is a regularizer, not dependent on the data
  - Fixed training set is a special case

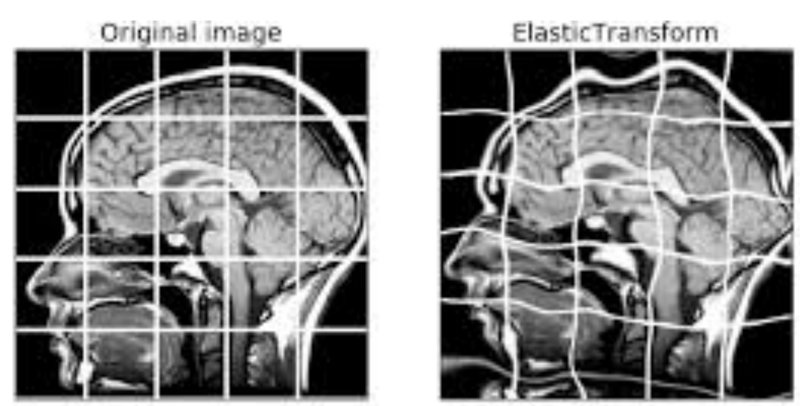
- SGD:
  - Draw a batch of data $(x_i, y_i)_{i=1}^{M}$ i.i.d. from p^*
  - $\tilde{g} = \frac{1}{M}\sum_i \nabla l(y_i, f(x_i, \theta)) + \nabla R(\theta)$

Data augmentation (Lecture 6)

rigid transforms



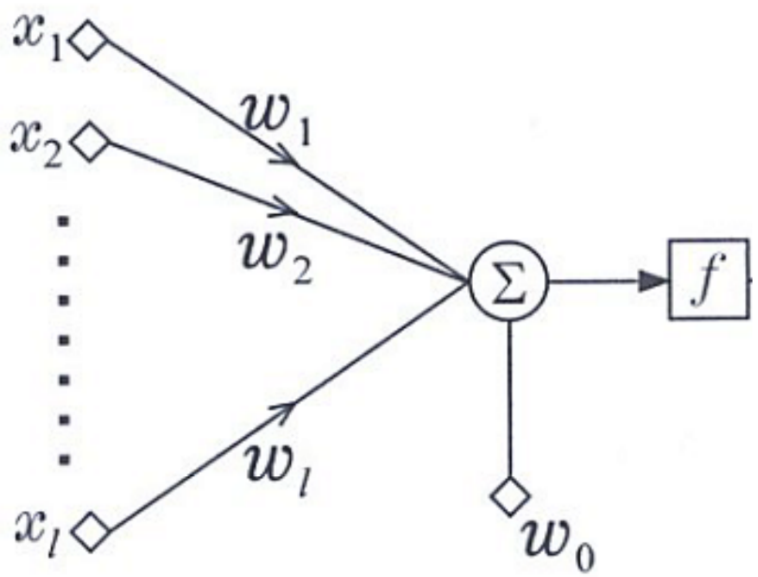
noise and distortions



rendering

Perceptron Algorithm

- Neural Network 1950s: Perceptron



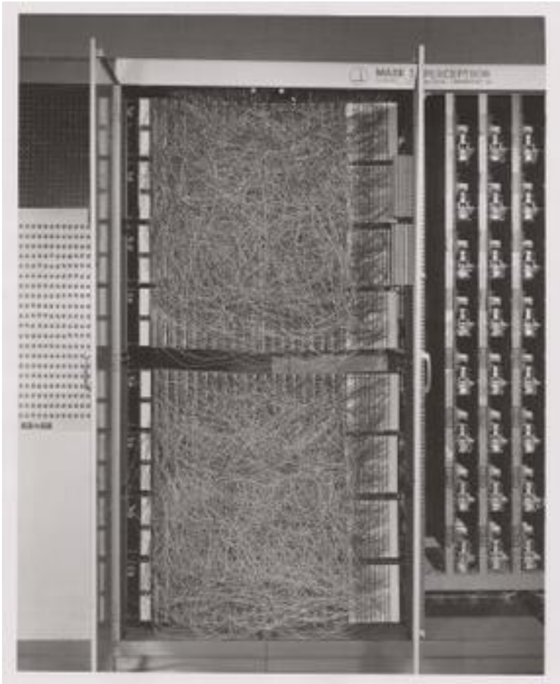
Press: "the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence"

Frank Rosenblatt

- Perceptron Algorithm as SGD:
  - Two classes $y = \pm 1$
  - Predictor: $f(x) = w^{\mathsf{T}} x$, decide by sign
  - Loss: $l(y, f(x)) = \max(-y w^{\mathsf{T}} x, 0)$
  - Draw a point (x, y) from the training data at random
  - Stochastic gradient: $\tilde{g}_t = \begin{cases} -yx, & \text{if classified incorrectly} \\ 0, & \text{otherwise} \end{cases}$
  - Make a step: $w_{t+1} = w_t + yx$
  - No need of step size thanks to scale invariance

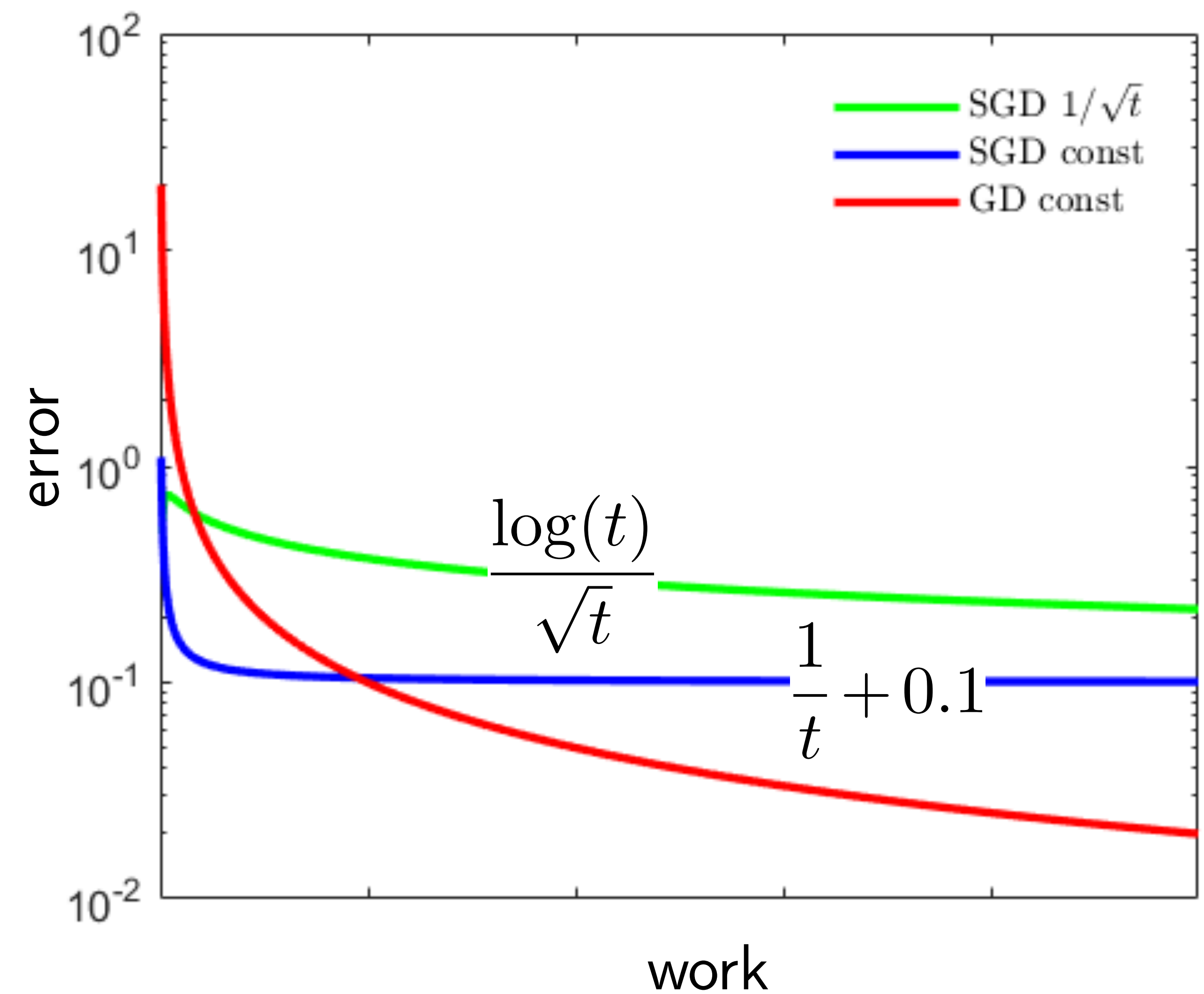
- First GPU:

Mark I Perceptron, 1958



Convergence Rates

- Iteration cost:
  - GD: $O(n)$ – full data
  - SGD: $O(M)$ – mini-batch
- Guarantees on convergence rate **depend on assumptions**. Setup closest to NNs:
  - $L(\theta)$ is bounded from below
  - $\nabla L(\theta)$ is Lipschitz continuous with constant ρ
  - Bounded variance: $\mathbb{E}\|\nabla l_i(\theta) - \nabla L(\theta)\|^2 \leq \sigma^2$
    or stronger condition $\mathbb{E}\|\nabla l_i(\theta)\|^2 \leq \sigma^2$ for some σ and all θ
- Convergence rates:
  - Error at iteration t: best over iterations expected gradient norm, $\min_{k=1\ldots t-1}\{\|\mathbb{E}[\nabla L(\theta_k)]\|\}$
  - GD with step size $\alpha_t = \alpha$
    Error: $O(\frac{1}{t})$
  - SGD with step size $\alpha_t = \alpha/\sqrt{t}$
    Error: $O(\frac{\log(t)}{\sqrt{t}})$
  - SGD with step size $\alpha_t = \alpha$
    Error: $O(\frac{1}{t}) + O(\alpha\rho\sigma^2)$



[Mark Smidt CPSC 540 Lecture 11]

Convergence Rates

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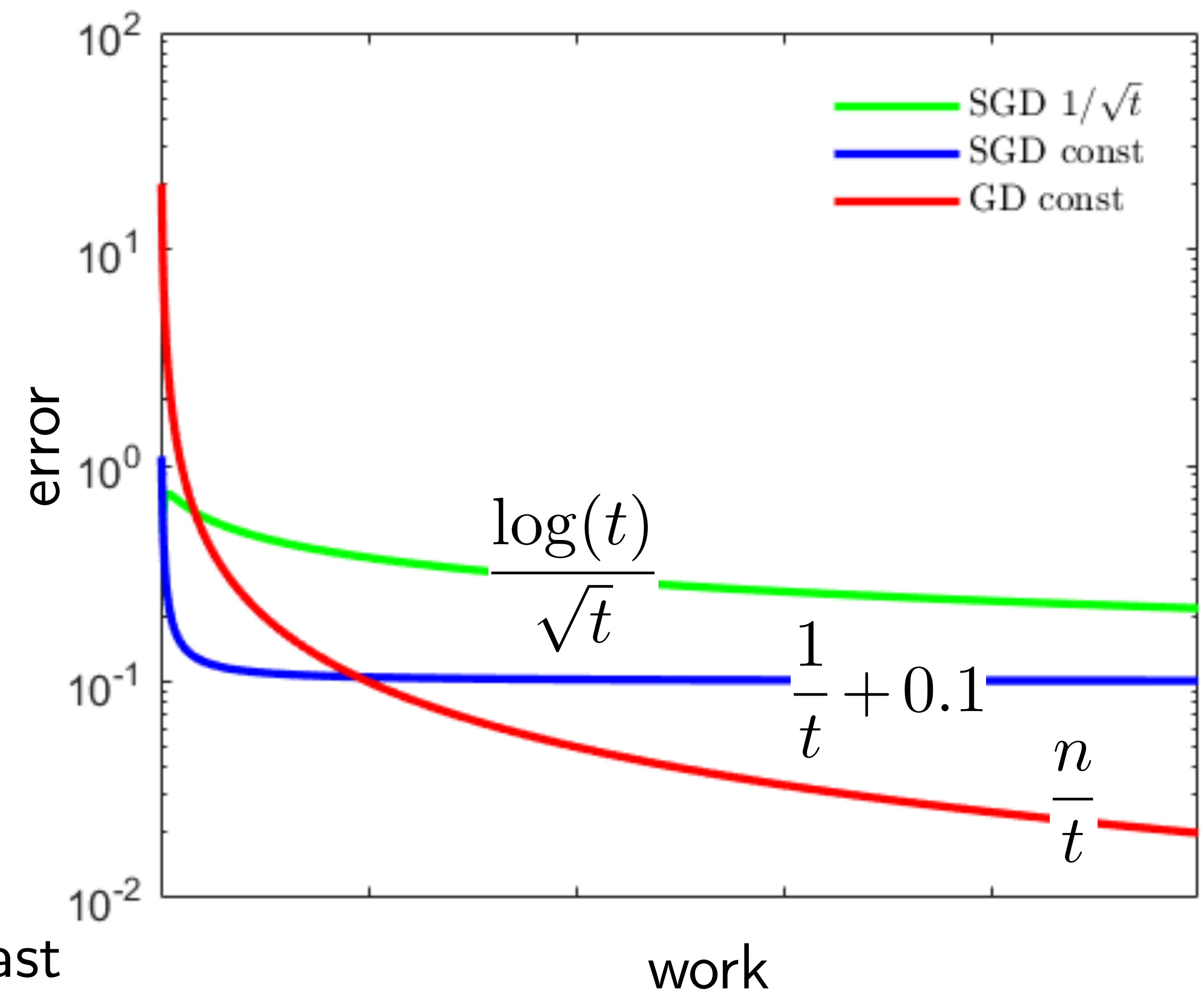

- Insights:
  - SGD wins when there is a lot of data
  - Convergence with a constant step size is fast but to within a “region” around optimum

- Remarks:
  - To have guarantees need to use conservative estimates with very small step sizes, etc.
  - Different other setups possible: convex / strongly convex, smooth/non-smooth
  - The rate is often faster in practice, but the general picture stays

Convergence Rates

- Convergence rates:
  - GD with step size $\alpha_t = \alpha$
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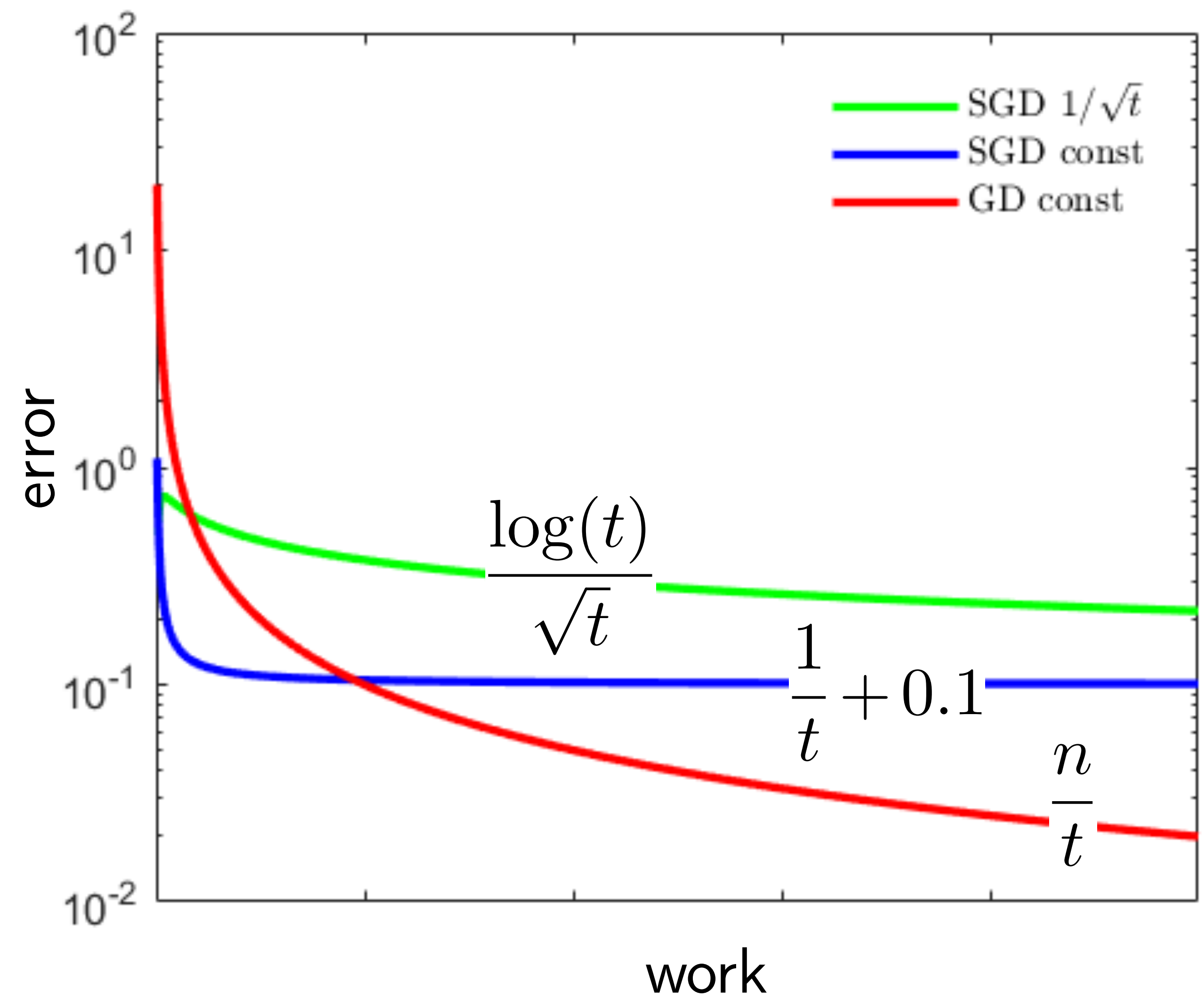
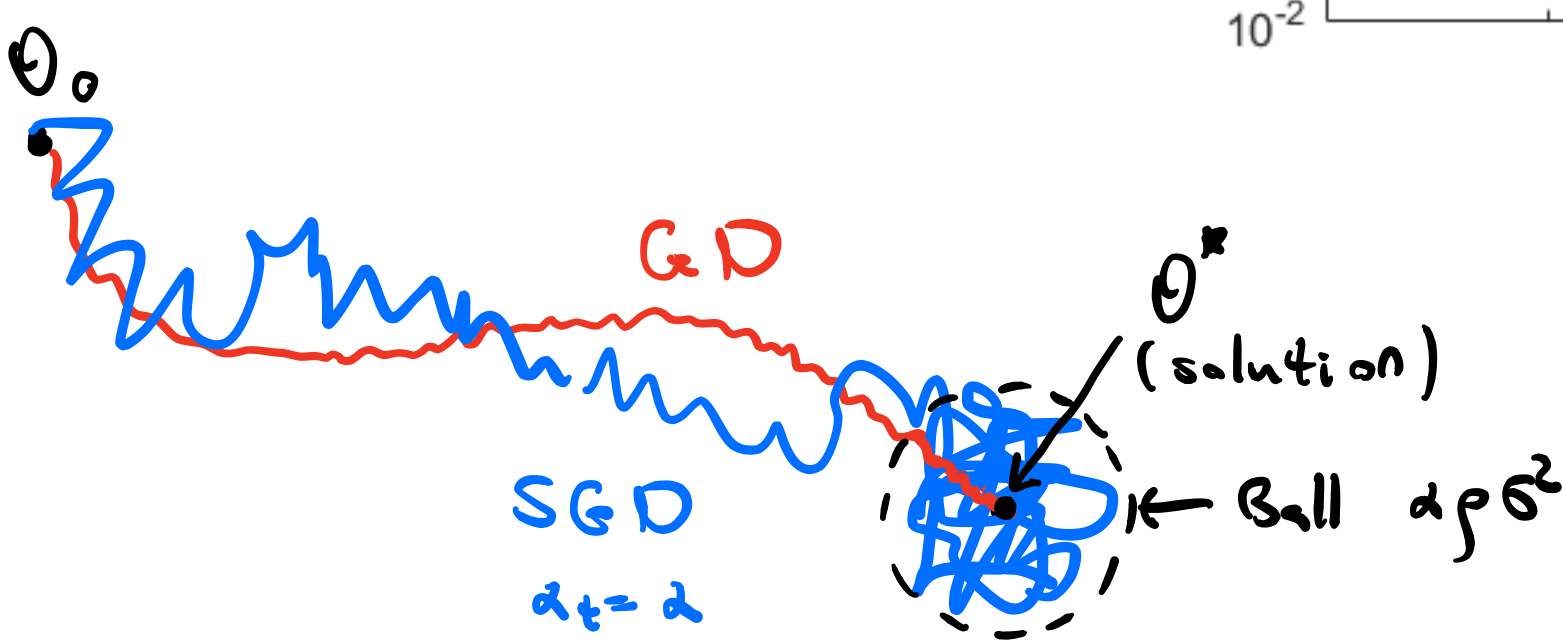
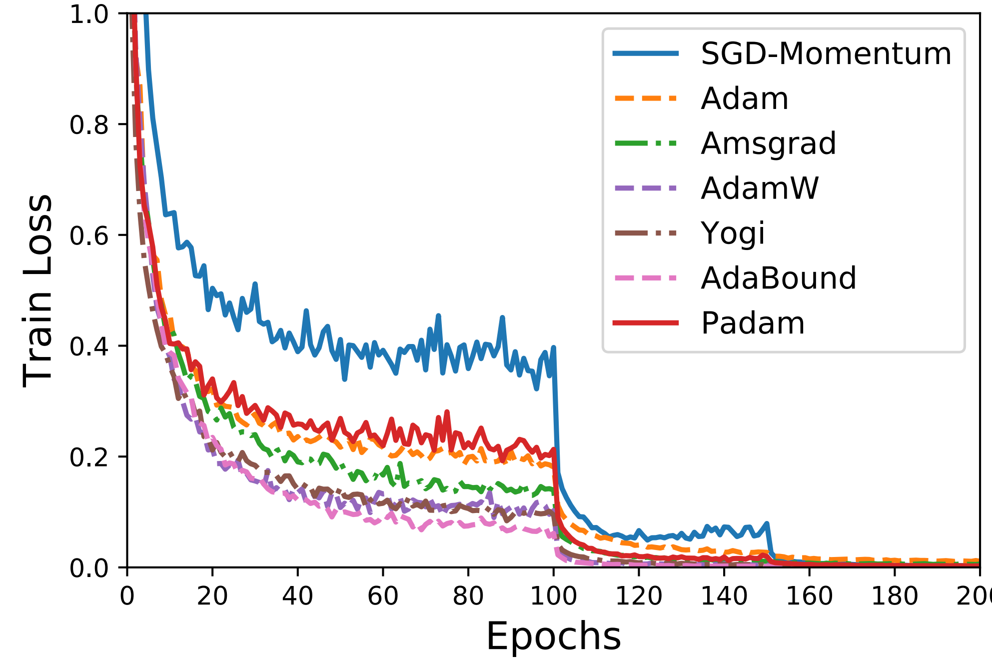




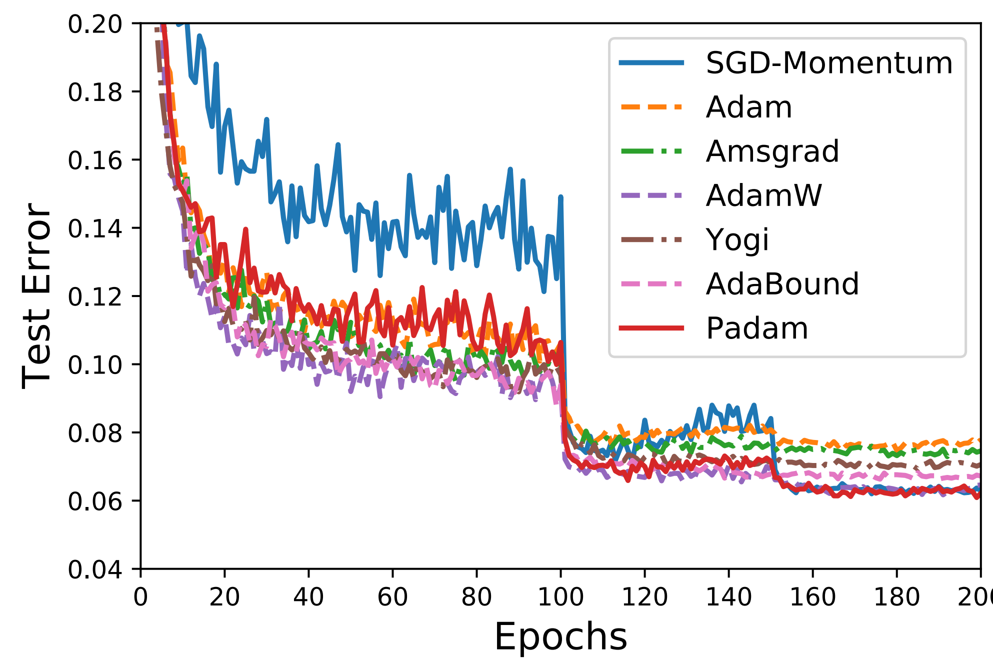
Learning Rate Schedule

- Common practice: decrease learning rate in steps
  - Example: start with $\alpha = 0.1$ then decrease by factor of 10 at epochs 100 and 150



(a) Train Loss for VGGNet

- Comments
  - Consistent with the idea of fast convergence to a region
  - After the sep size decrease, "1/n" rate replays
  - Many other empirically proposed schedules



(d) Test Error for VGGNet

Courtesy: [Chen et al. "Closing the Generalization Gap of Adaptive Gradient Methods in Training Deep Neural Networks"]

How to Draw Data Points?

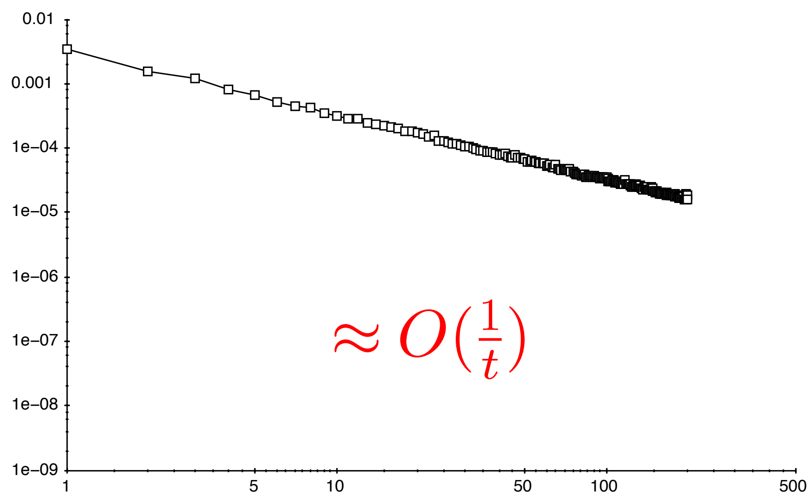
✦ How should we draw data points for SGD:

- every time select randomly with replacement
- shuffle the data once
- shuffle at each epoch but draw without replacement

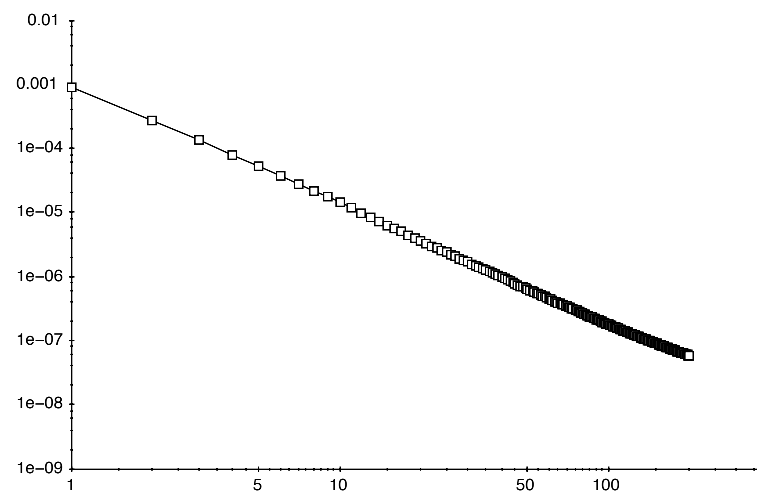
✦ Empirical evidence:

Bottou (2009): "Curiously Fast Convergence of some Stochastic Gradient Descent Algorithms"

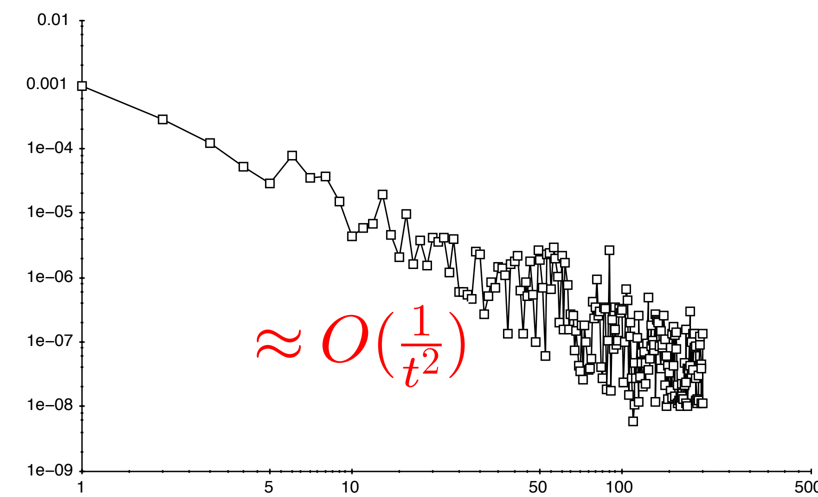
logistic regression $d = 47{,}152$, $n = 781{,}256$



Random selection: slope=−1.0003



Cycling the same random shuffle: slope=−1.8393



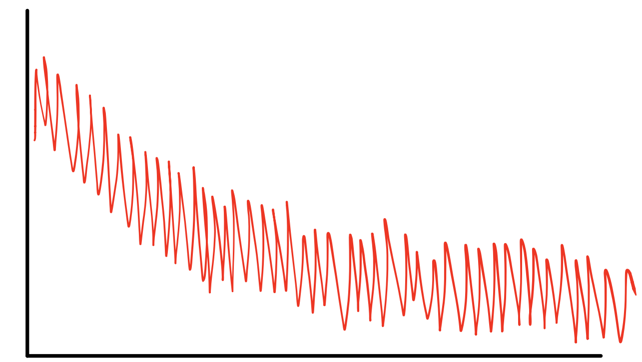
Random shuffle at each epoch: slope=−2.0103

◆ A simple consideration:

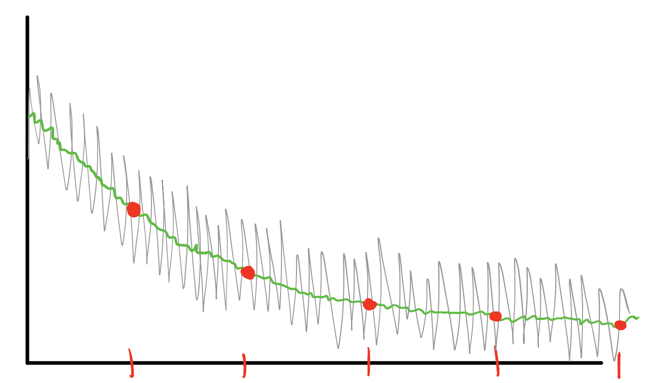
Drawing n times with replacement from the dataset of size n some points may not be selected. On average each point is selected with probability ≈ 0.63 for large n. Takes long time to even out ($\star$) – associated exercise

How to Measure the Progress?

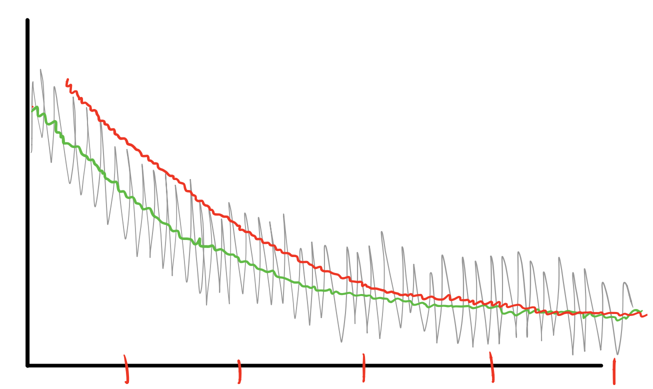
- ✦ Batch Estimate
  - Batch mean: $\tilde{L} = \frac{1}{M}\sum_{i \in I} l_i$
  - Not good idea, too high variance



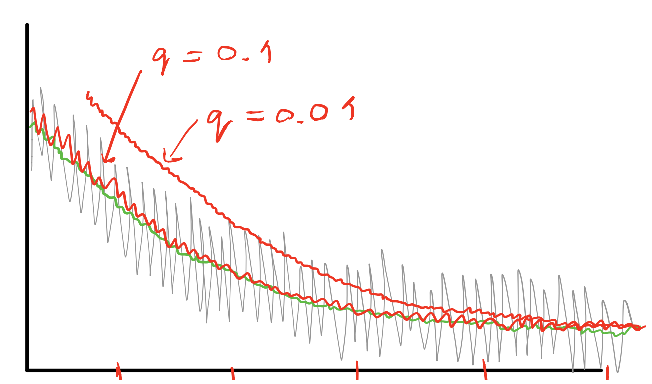
- ✦ Training data mean
  - $L = \frac{1}{n}\sum_i l_i$
  - Accurate, good if the dataset not too large



- ✦ Average using all last known loss values
  - $L := \frac{1}{n}\left(\sum_{i \in I} l_i^{\text{new}} + \sum_{i \notin I} l_i^{\text{old}}\right)$
  - Low variance, hysteresis 1 epochs
  - need to remember losses for full dataset



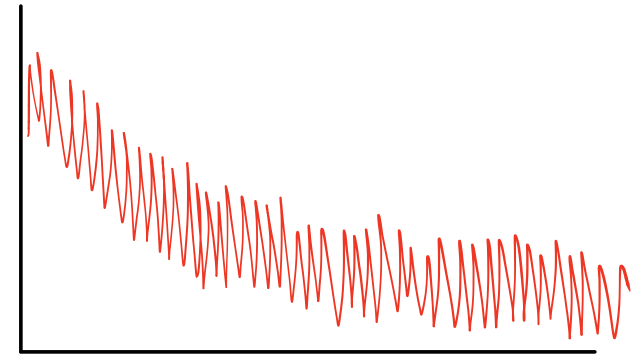
- ✦ Running Exponentially Weighted Average (**EWA**)
  - $L := (1-q)L + q\tilde{L}$
  - Higher variance/ larger hysteresis
  - remember only the running average loss



Same Applied to Gradient — Variance Reduction

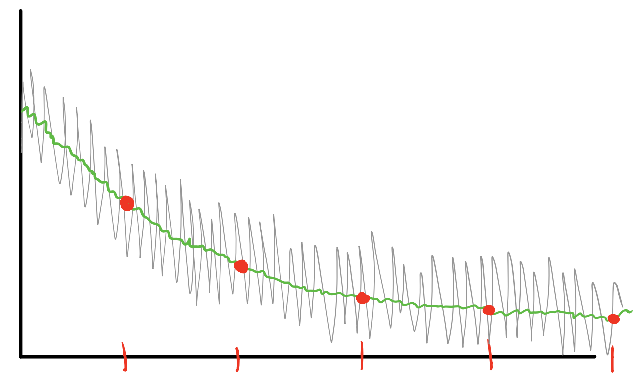
✦ SGD

- Batch mean: $\tilde{g} = \frac{1}{M}\sum_{i \in I} \nabla l_i$
- need a small step size



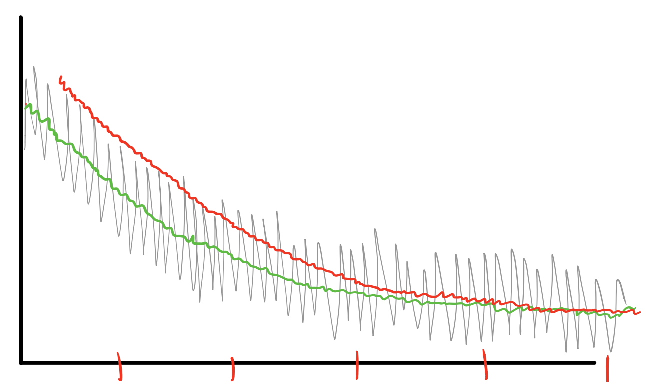
✦ GD

- Full gradient: $g = \frac{1}{n}\sum_i \nabla l_i$
- too costly



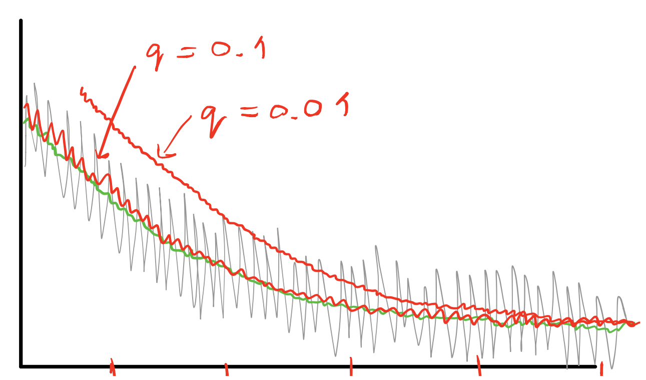
✦ Stochastic Average Gradient (**SAG**)

- $\tilde{g} := \frac{1}{n}\Big(\sum_{i \in I} (\nabla l_i)^{\text{new}} + \sum_{i \notin I} (\nabla l_i)^{\text{old}}\Big)$
- Improved convergence rates (convex analysis)
- need to remember gradients



✦ SGD with **momentum**

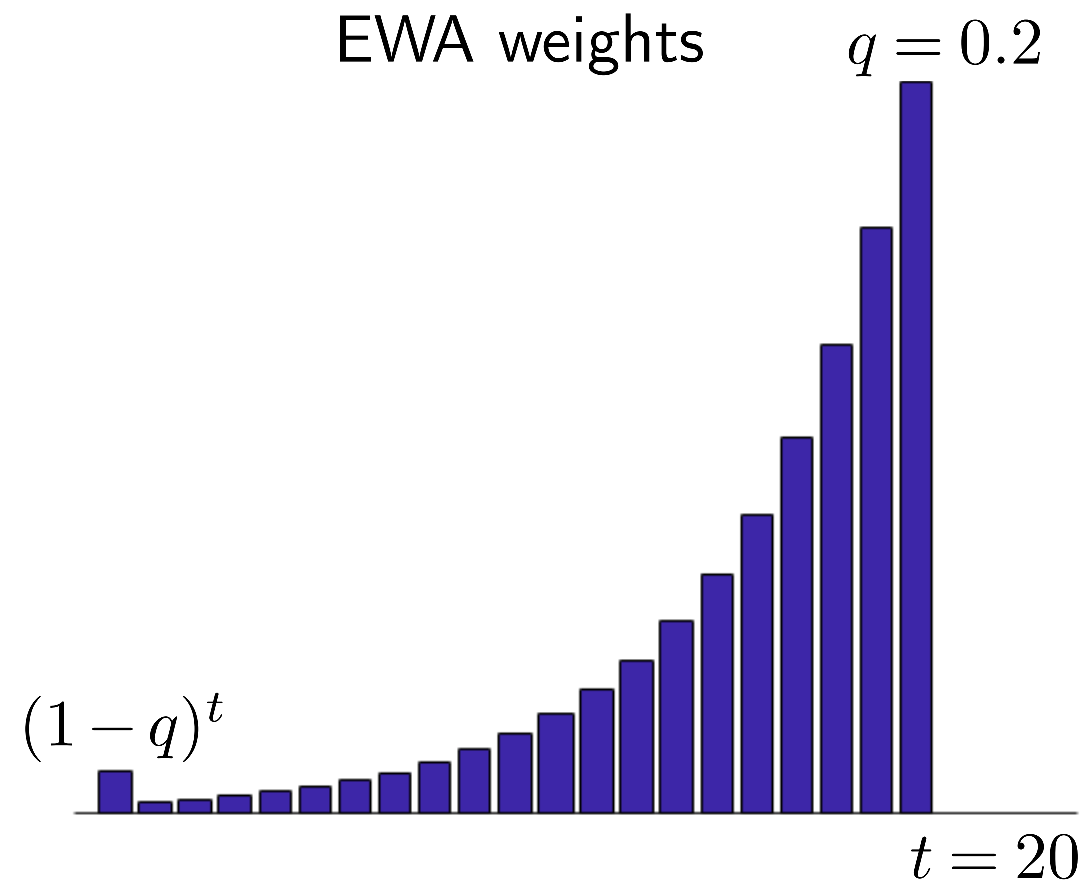
- $g := (1-q)g + q\tilde{g}$
- practical variance reduction
- remember only the running average gradient

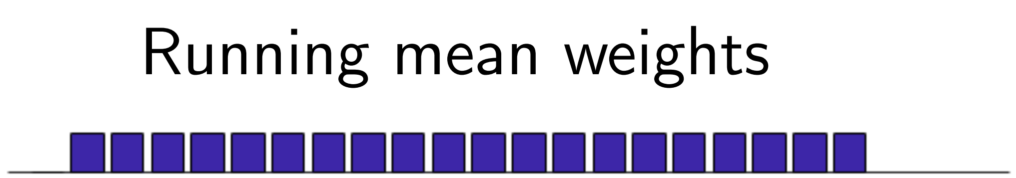


Running Averages

- General setup:
  - $X_k,\ k = 1, \ldots, t$ – independent random variables
  - $q_t \in (0, 1]$
  - Running mean: $\mu_t = (1 - q_t)\mu_{t-1} + q_t X_t$
- Exponentially Weighted Average (**EWA**):
  - Constant $q_t = q$
  - $\mu_1 = (1 - q)\mu_0 + qX_1$
  - $\mu_2 = (1 - q)^2\mu_0 + (1 - q)qX_1 + qX_2$
  - $\ldots$
  - $\mu_t = (1 - q)^t\mu_0 + \sum_{1 \le k \le t} (1 - q)^{t-k} qX_k$

$$= w_0\mu_0 + \sum_{1 \le k \le t} w_k X_k$$





- **Running mean**:
  - $q_t = \frac{1}{t}$
  - $\mu_1 = 0\mu_0 + X_1$
  - $\mu_t = \frac{t-1}{t}\mu_{t-1} + \frac{1}{t}X_t$
  - $\mu_{t+1} = \frac{t}{t+1}\mu_t + \frac{1}{t+1}X_{t+1} = \frac{t-1}{t+1}\mu_{t-1} + \frac{1}{t+1}\left(X_t + X_{t+1}\right)$

($\star$) Smooth transition from running mean to EWA

SGD with Momentum

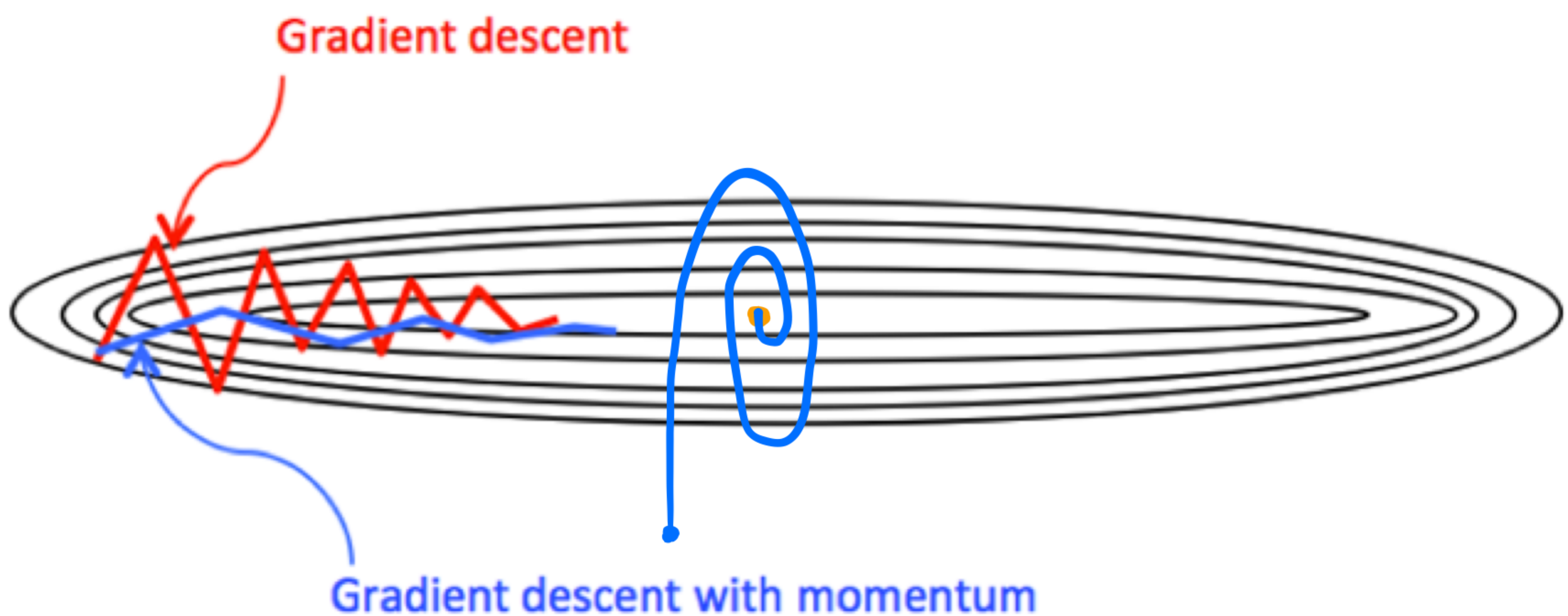
- Algorithm
  - Stochastic gradient: $\tilde{g} = \frac{1}{M}\sum_{i \in I_t} \nabla l_i$
  - EWA gradient: $g_t = (1-q)g_{t-1} + q\tilde{g}$
  - Step: $\theta_t = \theta_{t-1} - \alpha g_t$
- Can rewrite in different forms, e.g. in pytorch:
  - Velocity: $v_t = \mu v_{t-1} + \tilde{g}$
  - Step: $\theta_t = \theta_{t-1} - \varepsilon v_t$

($\star$) Equivalent by setting: $v_t = g_t/q$, $\mu = (1-q)$, $\varepsilon = q\alpha$

- When changing momentum μ often need to adjust the learning rate as well

SGD with Momentum

- With variance sufficiently low → GD with momentum, *i.e.* consider $\tilde{g}$ is noise-free
  - Velocity: $v_t := \mu v_{t-1} + \tilde{g}$
  - Step: $\theta_t = \theta_{t-1} - \varepsilon v_t$
- Even exact gradient may not be a good direction
- Cancels "noise" in the incorrect prediction of the function change



- The **"heavy ball"** method
  - Friction ($\mu < 1$) and slope forces build up velocity
  - Recall the hysteresis effect from using estimates from the past
  - The inertia may lead to oscillatory behavior (not good)
  - Sometimes helpful to overcome plateaus

★ "Nesterov" Momentum

- Common Momentum
  - Velocity: $v_{t+1} = \mu v_t + \tilde{g}(x_t)$
  - Step: $x_{t+1} = x_t - \varepsilon v_{t+1}$

The step consists of momentum and current gradient

The momentum part of the step is known in advance

Can make it before computing the gradient:

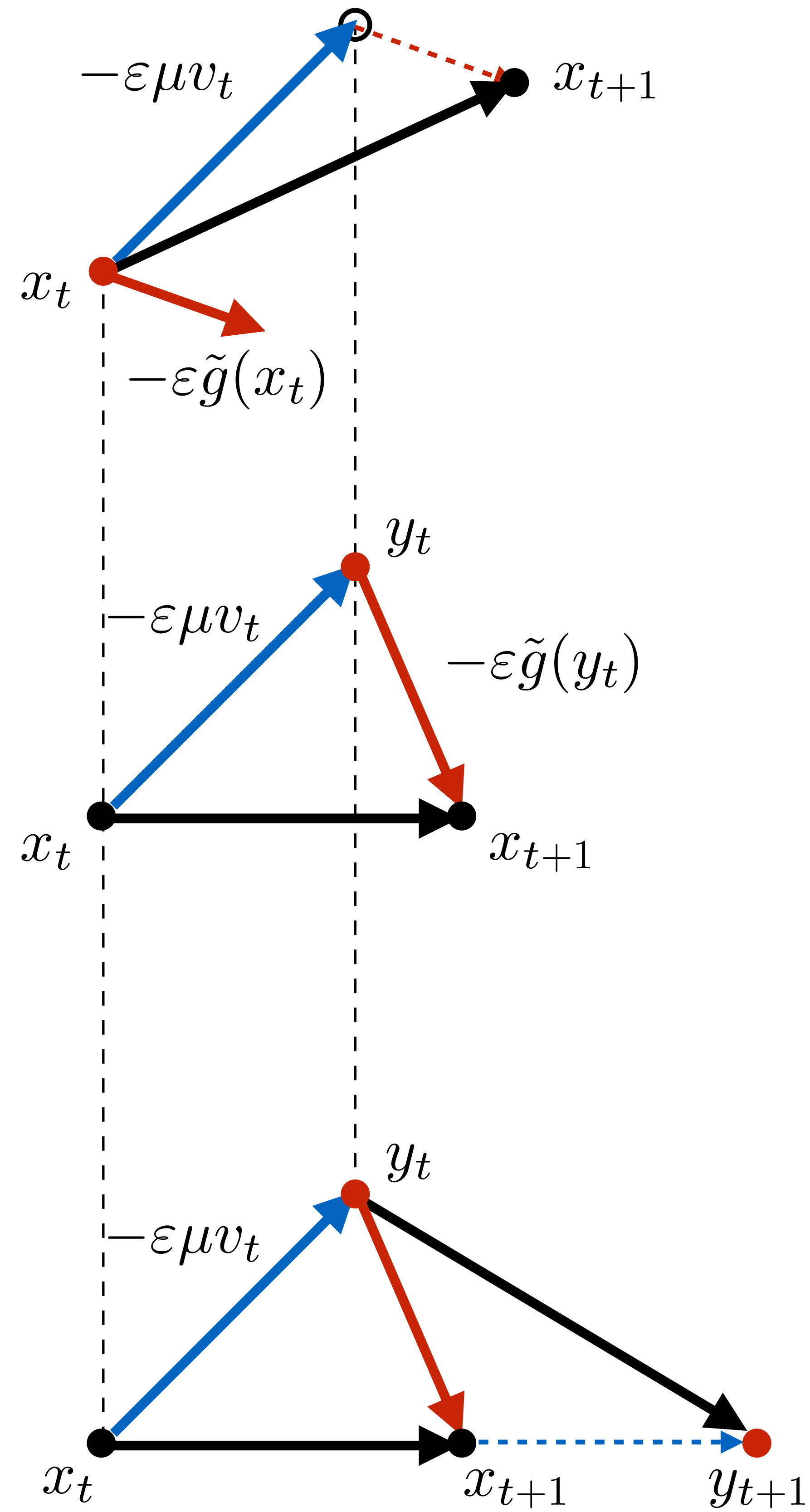
- Nesterov Momentum
  - Leading sequence: $y_t = x_t - \varepsilon \mu v_t$
  - Velocity: $v_{t+1} = \mu v_t + \tilde{g}(y_t)$
  - Step: $x_{t+1} = y_t - \varepsilon \tilde{g}(y_t)$

Takes advantage of the known part of the step

Less overshooting

- Can express as steps on the leading sequence alone ($\star$):
  - Velocity: $v_{t+1} = \mu v_t + \tilde{g}(y_t)$
  - Step: $y_{t+1} = y_t - \varepsilon\big(\tilde{g}(y_t) + \mu v_{t+1}\big)$

The two sequences eventually converge



★ Running Averages: How Much Smoothing?

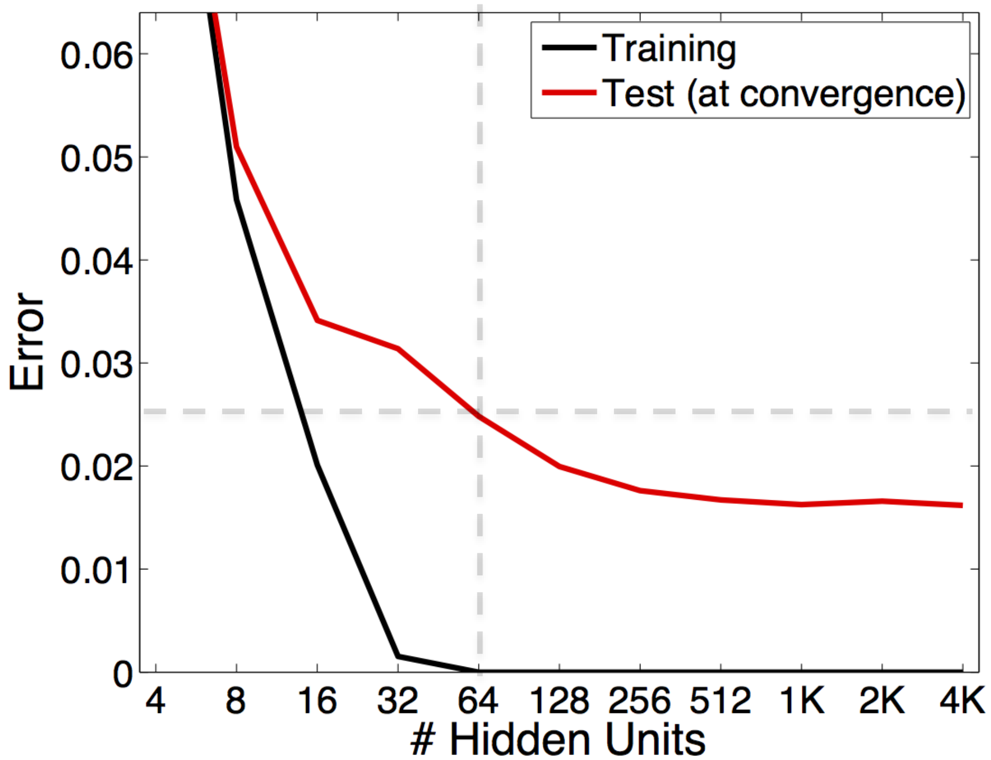
- General setup
  - X_t – independent random variables
  - $q_t \in (0, 1]$
  - Running mean: $\mu_t = (1 - q_t)\mu_{t-1} + q_t X_t$ is a r.v.
- Expectation:
  - $\mathbb{E}[\mu_t] = (1 - q_t)\mathbb{E}[\mu_{t-1}] + q_t \mathbb{E}[X_t]$ – running average of expectations
  - $\mathbb{E}[\mu_t] = w_0 \mathbb{E}[\mu_0] + \sum_{k=1}^{t} w_k \mathbb{E}[X_k]$
  - When iterations stabilize (θ does not change much) an unbiased estimate
- Variance:
  - $\mathbb{V}[\mu_t] = (1 - q_t)^2 \mathbb{V}[\mu_{t-1}] + q_t^2 \mathbb{V}[X_t]$
  - $\mathbb{V}[\mu_t] = w_0^2 \mathbb{V}_0 + \sum_{k=1}^{t} w_k^2 \mathbb{V}[X_k]$
  - Variance reduction of running mean: $\sum_{k=0}^{t} w_k^2 = \sum_{k=1}^{t} \frac{1}{t^2} = \frac{1}{t}$
  - Variance reduction of EWA: $\sum_{k=0}^{t} w_k^2 = \frac{q^2}{1-(1-q)^2}$ – in the limit of large t

($\star$) Equivalent window size of EWA: $n = \frac{2}{q} - 1$. E.g. $q = 0.1 \leftrightarrow n = 19$

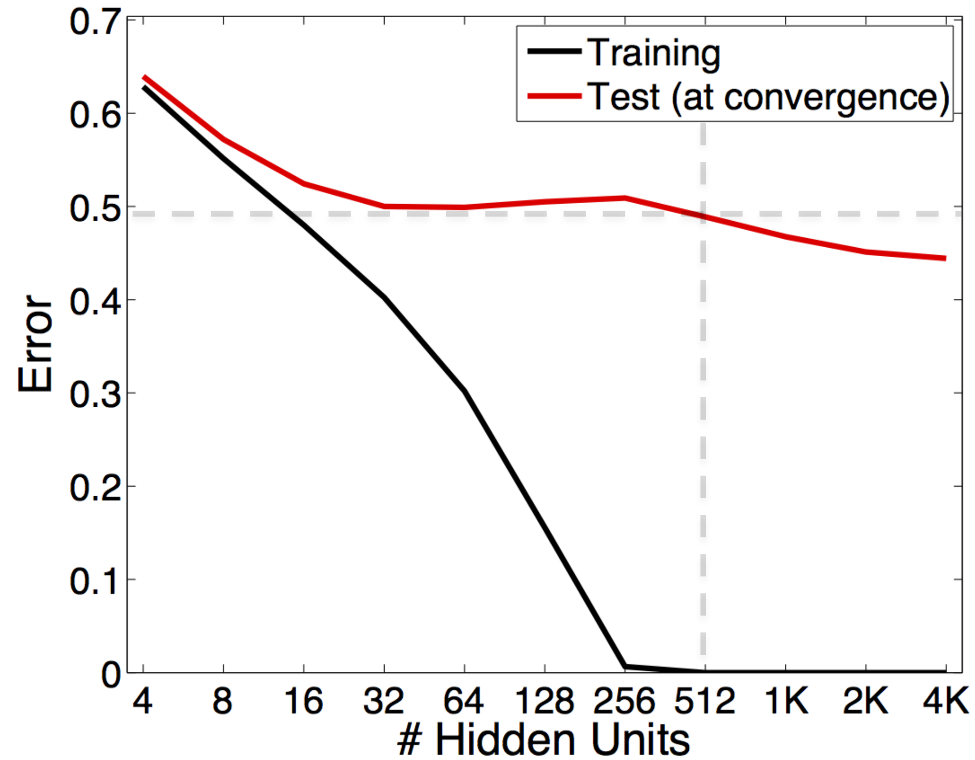
- Can use EWA with a decreasing q series for a progressive smoothing

Implicit Regularization

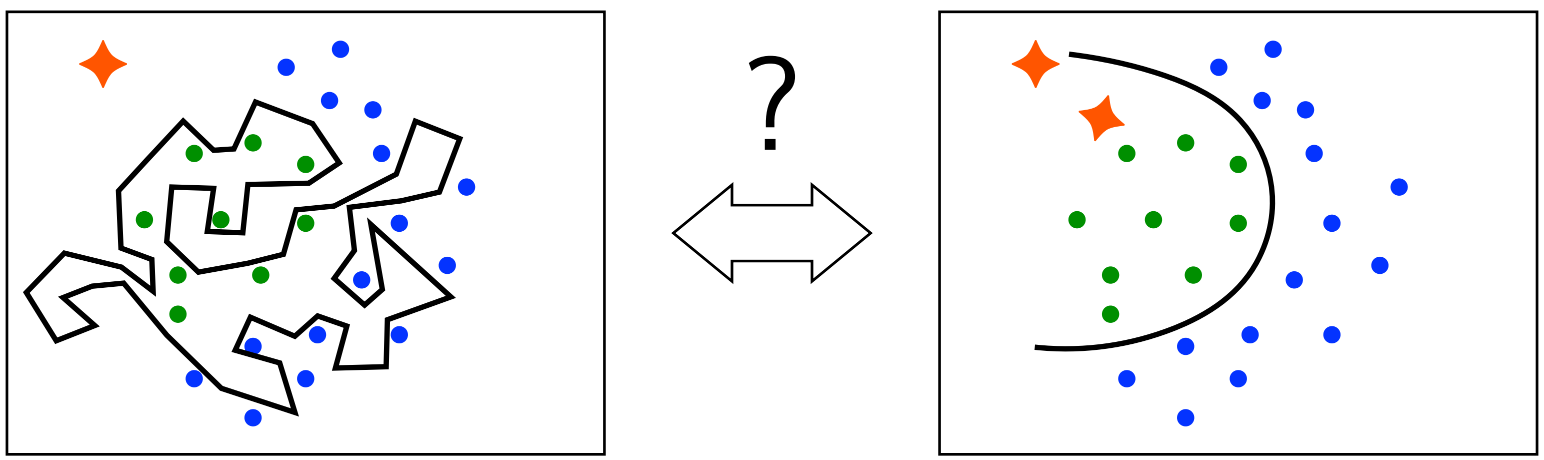
MNIST



CIFAR-10



- We increase the network capacity but generalization improves, why?
  - There exist global minima that do not generalize
  - SGD somehow finds a good global minimum



★ Implicit Regularization: Min. Norm

- Linear models:
  - The model is linear: $f(x) = w^\mathsf{T} x$
  - Training loss: $L = \sum_{i=1}^{n} l(w^\mathsf{T} x_i, y_i)$
  - Loss has a unique finite root: $l(y, y_i) \geq 0$ with equality iff $y = y_i$

  Theorem (Gunasekar et al. 2018) If iterates of SGD start with w_0 and converge to a solution w_∞ that is a global minimizer of L, then

$$w_\infty = \arg\min_{w \in \mathcal{W}} \|w - w_0\|^2,$$

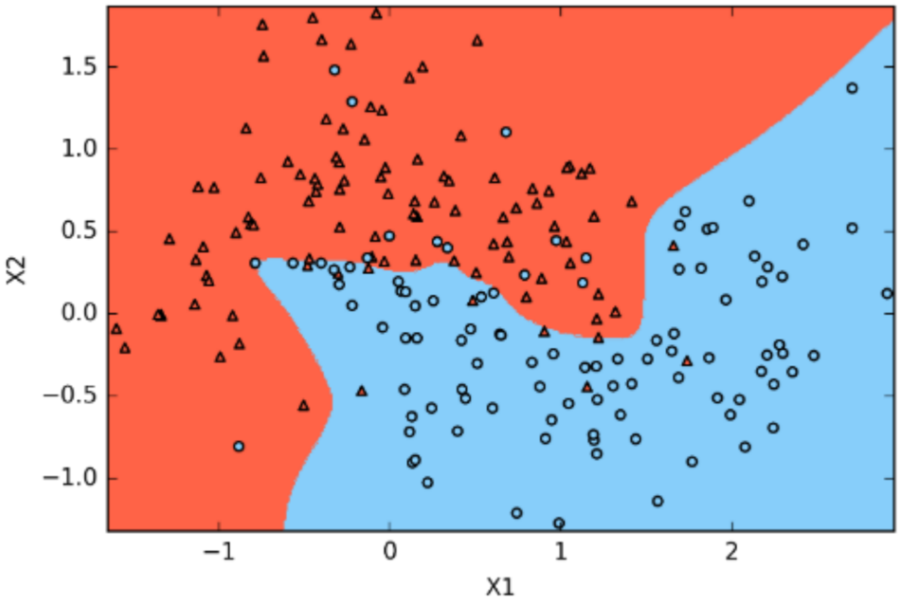
  where $\mathcal{W}$ is the solution space: $\mathcal{W} = \{w | (\forall i) w^\mathsf{T} x_i = y_i\}$.

- Remarks:
  - We do observe convergence to global minima in practice (overparameterized models)
  - Some recent theoretical and experimental results indicating this extends to deep networks
  - So even without explicit l2 norm regularization SGD does some of that implicitly

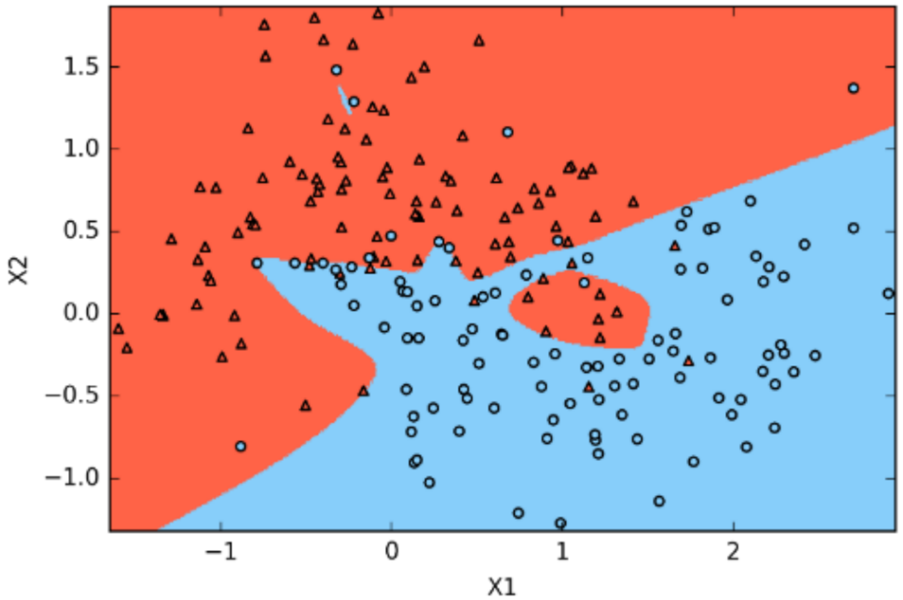
★ Implicit Regularization: Batch Size

- Typically choose batch size to fully utilize parallel throughput (in GPUs means ~10^4 independent arithmetic computations in parallel)
- Limited by memory
- Smaller batch -> noisier gradient -> implicit regularization

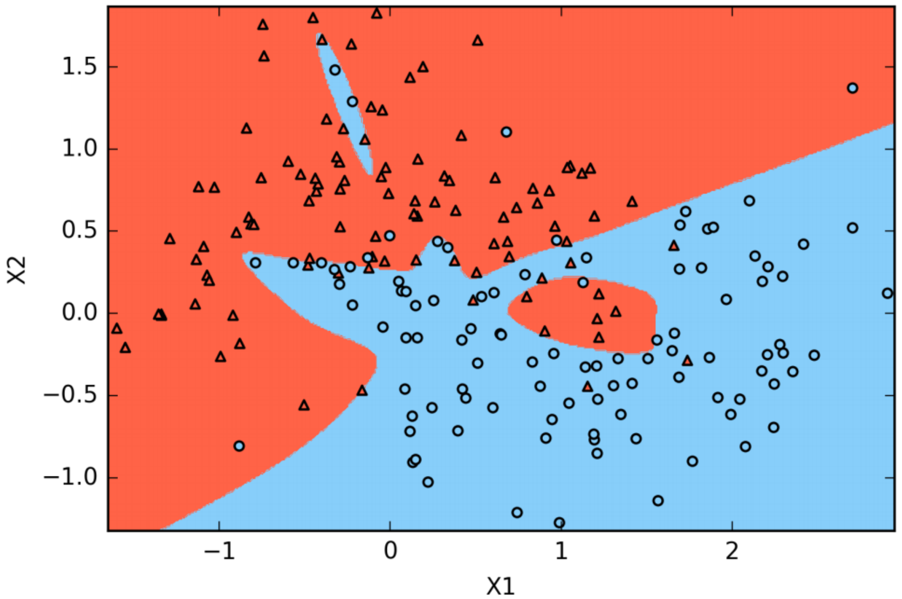
Synthetic data



Decision boundary of batch size 1

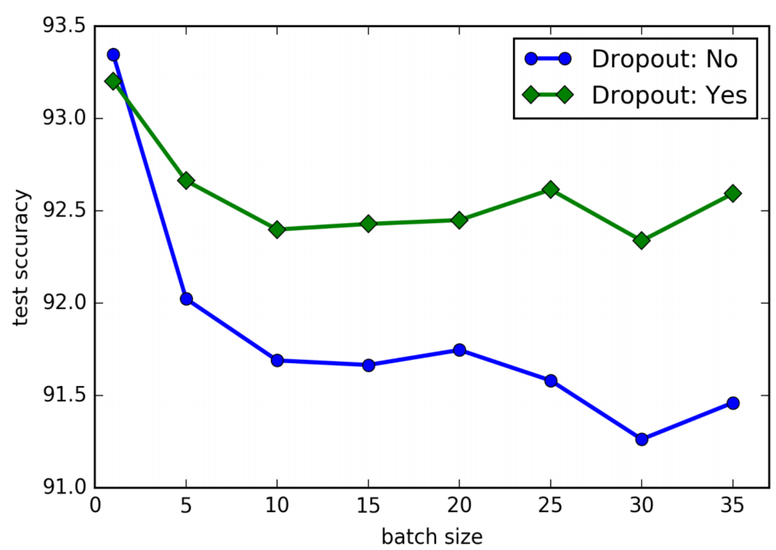


Decision boundary of batch size 5



Decision boundary of batch size 30

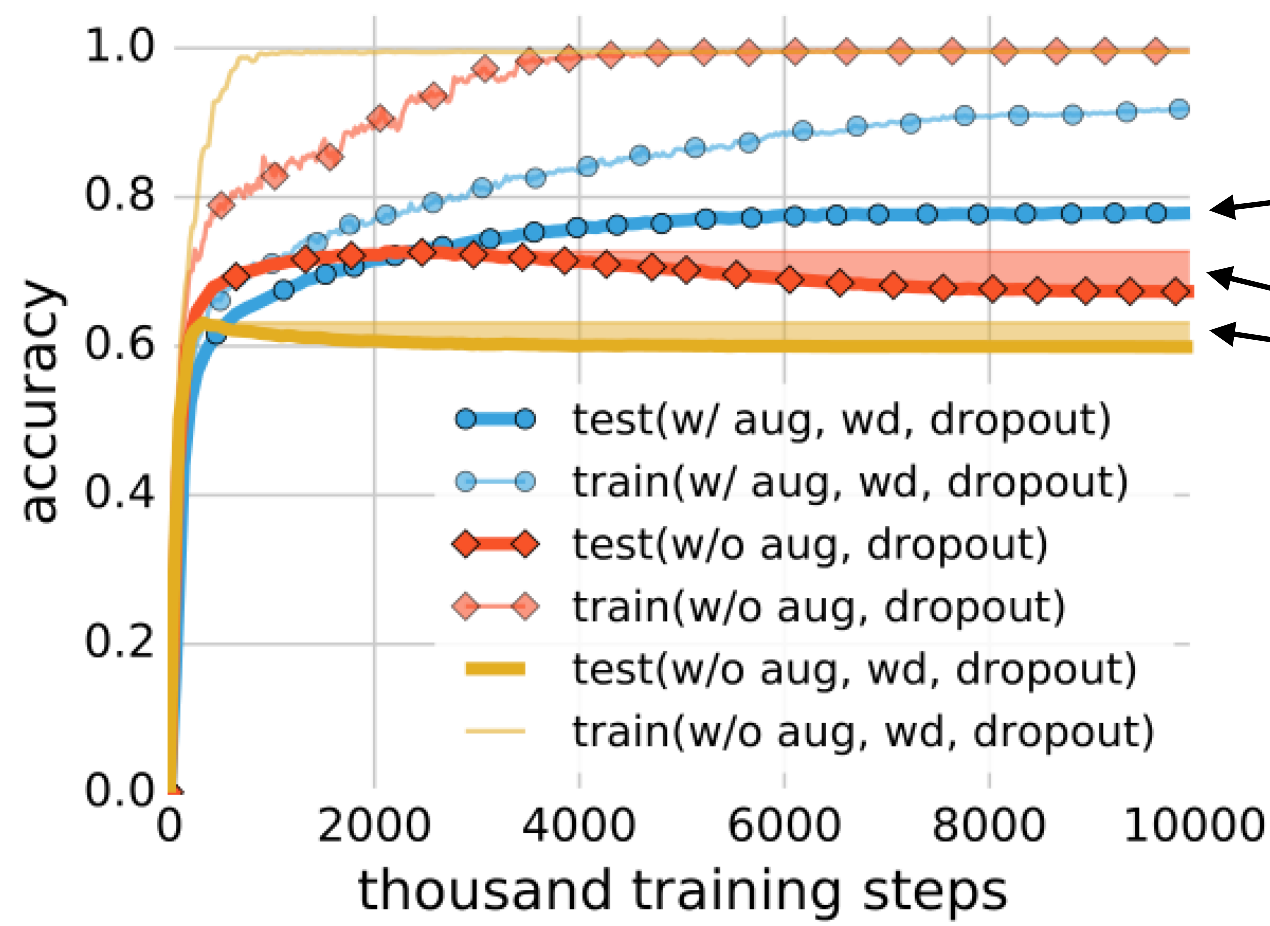
NLP data



Lei et al. (2018) "Implicit Regularization of Stochastic Gradient Descent in Natural Language Processing: Observations and Implications"

★ Implicit Regularization: Early Stopping

- ✦ We expect the learning to overfit, often it does not
- ✦ Example when it does:



(a) Inception on ImageNet

explicit regularization

no overfitting

Test accuracy decreases with more iterations

[Zhang et al. (2017) "Understanding Deep Learning Requires ReThinking Generalization"]

- ✦ Early stopping could potentially improve generalization when other regularizers are absent
- ✦ Need a validation set

More in Lecture 8

- Loss Landscape of NNs
  - Permutation invariance and overcomplete parameterizations
  - Local minima and saddle points in high dimensions
  - Empirical evidence of many good local minima
  - Redundancy helps optimization
- SGD sensitivity to change of variables
- Adaptive methods
- Handling simple constraints - Mirror Descend