Optimization

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Loss functions

1948 US Presidential election won by… Harry Truman

$$L_{0-1}(winner = Dewey) = 1$$

0-1 loss well suited to classification

Loss function: Penalty for when we get it wrong

examples:

- 0-1 loss $L_{0-1}(\hat{y}) = \begin{cases} 0 & \hat{y} = y \\ 1 & \hat{y} \neq y \end{cases}$
- MSE $L_{MSE}(\hat{y}) = (\hat{y} - y)^2$

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Risk

- When optimizing, we are not so concerned with the loss of an individual example
- Goal is to minimize the expected loss which is known as the risk

$$J^*(\theta) = E_{(x,y) \sim p_{data}}[L(f(x \mid \theta), y)]$$

where p_{data} is the actual (and probably unknown) distribution of the data.

Empirical risk

- Since we do not have p_{data} we usually use a training set, $\hat{p}_{data}$, and compute the *empirical risk* using the sample expected value:

$$J(\theta) = E_{(x,y) \sim \hat{p}_{data}}[L(f(x \mid \theta), y)]$$

Optimizers and classification

- $L_{0\text{-}1}$ makes sense for classification, but what if we want to minimize it?

$$L_{0-1}(\hat{y}) = \begin{cases} 0 & \hat{y} = y \\ 1 & \hat{y} \neq y \end{cases} \qquad \nabla L_{0-1}(\hat{y})\,?$$

- Difficult to minimize… leads us to *surrogate loss* functions that are easy to optimize

Surrogate loss functions

- We have already seen a couple
  - cross entropy
  - negative log likelihood for binary classifiers
- Advantages
  - easier to optimize
  - can continue to learn *even when empirical loss is 0*
    - might be good: can learn to better distinguish between classes
    - might be bad: can lead to overfitting

Batch learning

1. Compute gradient for each example & target in the *entire training set*
2. Update model in mean gradient direction
3. Go to 1 if not done

- Tends to have a good estimate of the gradient (standard error of mean estimator is $\sigma/\sqrt{n}$)
- Learns slowly

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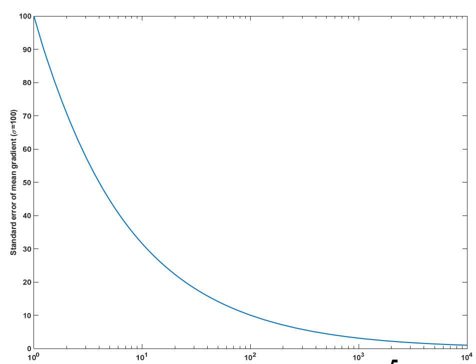
Stochastic, or minibatch learning



- Standard error driven by $\sigma/\sqrt{n}$
- Implies diminishing gains as *n* grows

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Stochastic, or minibatch learning

We can have a small number of examples and achieve decent estimates of the gradient.

Noise in the gradient estimate can serve as a regularizer.

Batch size considerations

- Too small – Underutilizes parallel hardware
- Too large –Excessive memory demands, slow learning

Stochastic batch size

- Gradient only algorithms – small batch sizes okay (e.g. 100)
- Algorithms that rely on Hessians require more data to estimate (e.g. 10,000)

Stochastic learning

- Samples are assumed to be independent
- If not, can produce a biased estimator of the loss surrogate and its gradient
- Many data sets have correlated samples; batches from such sets should be sampled randomly

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Challenges in optimization

- Ill-conditioned Hessians can wreak havoc

oh, oh…
rabbit hole

British Postal Service, Graham Baker-Smith 2015

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Matrix condition numbers

- We have seen that some matrices have eigendecompositions

$A = Q\Lambda Q^T$ where $diag(\Lambda) = \lambda$, Q contains eigen vectors, and $QQ^T = I$

- More generally, every real matrix has a singular value decomposition

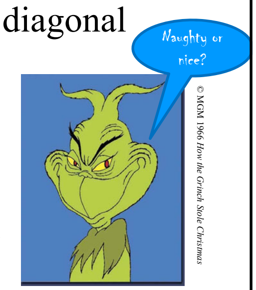
Singular value decomposition (SVD)

$$A = UDV^T$$

- A is $m \times n$
- U is $m \times m, V$ is $n \times n$
- D is diagonal and its elements along the diagonal are known as singular values

SVD is important for

- computing pseudo-inverses
- determining if matrices are well behaved



SVDs and condition numbers

- Condition number $\triangleq \frac{\max_i(D_{i,i})}{\min_i(D_{i,i})}$
- When the condition number is large, small changes in the input can produce large changes in the output

Ill conditioned Hessians can wreak havoc

A 2nd order Taylor-series expansion of the cost function shows

$$f(x^{(0)} - \epsilon g) \approx f(x^{(0)}) - \epsilon g + \frac{1}{2}\epsilon^2 g^T H g \quad \text{(Goodfellow et al. 4.9)}$$

so when H is ill conditioned, even smaller values of ϵ can cause us to overshoot and increase the cost. Learning rate must be shrunk in this case.

Ill-conditioned Hessians can wreak havoc

To determine if an ill-conditioned Hessian is a problem, monitor:

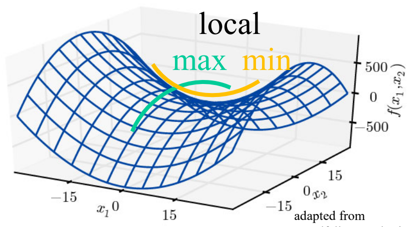
- squared gradient $g^T g$
- and $g^T Hg$

Challenges continued

- Local minima
  – Not usually a problem
  – Many local minima have similar valued cost functions
  – However, it is always possible that the global minimum is much lower

Challenges continued – saddle points

- Hessian's eigen values drive loss
- Moving along eigen vectors with
  - + eigen values increase cost
  - - eigen values decrease cost



adapted from Goodfellow et al. Fig 4.5

All + → local min
All - → local max

Saddle points

- In low dimensions, random functions typically have local minima
- In high dimensions, local minima are rare, but saddle points are common
  (saddle points : local minima ratio grows exponentially with dimensionality)

Saddle points

- Theory suggests that saddle points tend to be high cost, so how we handle them is important.
- Gradients at saddle points can be shallow
- First order gradient descent tends to escape many saddle points
- Some techniques try to find points where the gradient is zero (e.g. Newton's method). This can be problematic.

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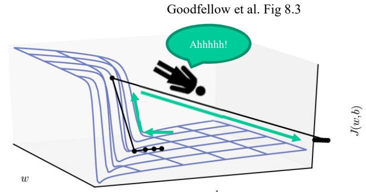
Challenges continued

- Plateaus
  - Wide flat regions. Problematic for all numerical optimization algorithms
- Cliff structures
  - Very steep gradients can result in large jumps
  - Gradient clipping prevents this from occurring (max norm for step size)

Goodfellow et al. Fig 8.3



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Challenges continued

- Long-term dependencies
  (we will discuss this when we cover recurrent neural nets)

- Inexact gradients
  Just like the distributions we learn, these are only approximations…

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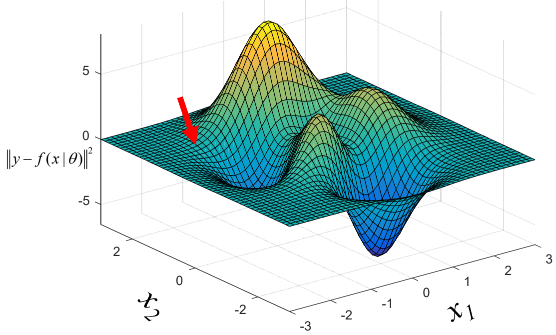
Challenges continued

- Our local point in optimization space may just not be a good one…



Ways to cope:
- non-local moves (e.g. simulated annealing)
- find a good starting point (current research direction)

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Stochastic gradient descent (SGD)

Given learning rate ϵ

while stop criterion not met

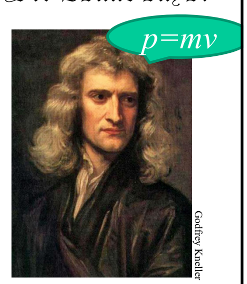
  randomly select m examples & labels (x, y)

  estimate gradient $\hat{g} = \frac{1}{m} \nabla_\theta \sum_i L(f(x^{(i)} \mid \theta), y^{(i)})$

  update model $\theta = \theta - \epsilon \hat{g}$

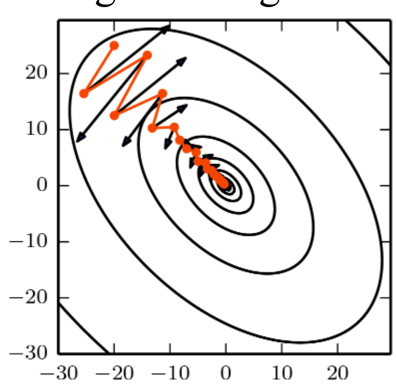
Common to diminish learning rate over time with time specific ϵ_t

Sir Isaac says:



Momentum

- Key idea: Use previous gradients to keep us moving in the right direction.



Black gradient vectors grow due to a poorly conditioned Hessian

SGD with momentum

Given learning rate ϵ and initial velocity v

while stop criterion not met

randomly select m examples & labels (x, y)

estimate gradient $\hat{g} = \frac{1}{m}\nabla_\theta \sum_i L(f(x^{(i)} \mid \theta), y^{(i)})$

update velocity $v = \alpha v - \epsilon \hat{g}$

update model $\theta = \theta + v$

Nesterov momentum variant: $\hat{g} = \frac{1}{m}\nabla_\theta \sum_i L(f(x^{(i)} \mid \underbrace{\theta + \alpha v}_{\text{apply momentum to model when estimating gradient}}), y^{(i)})$

(Doesn't help that much with SGD, but does in other cases.)

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Parameter initialization

- Key goal: break symmetry between units
- Most initialization based on heuristics
  - biases usually small constants
  - weights from uniform or Gaussian distributions
    - scale seems to be important
    - distribution family does not
  - see Goodfellow et al. for a variety of strategies

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Adaptive learning rates

- Learning rate has a large impact on success of neural networks
- Several algorithms have attempted to adapt the learning rates automatically
- RMSProp – Learning rate weighted by a function of moving average of gradients

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RMSProp

Given learning rate ϵ, decay rate ρ, $r = 0, \delta = 10^{-6}$

while stop criterion not met

randomly select m examples & labels (x, y)

estimate gradient $\hat{g} = \frac{1}{m}\nabla_\theta \sum_i L(f(x^{(i)} \mid \theta), y^{(i)})$

accumulate gradient[2] $r = \rho r + (1-\rho)\hat{g} \odot \hat{g}$

update model $\theta = \theta - \frac{\epsilon}{\sqrt{\delta + r}} \odot g$

$\odot$ element by element multiplication

$\sqrt{\delta + r}$ element by element root

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Adaptive moments (Adam)

- Moments of a random variable are its expected value raised to the n^th power:
$$E[X], E[X^2], \ldots, E[X^n]$$
- Adam uses leaky estimates of the first two moments of the gradient, giving it characteristics of both SGD with momentum and RMSProp

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Adam

Given step size ϵ, decay $\rho_1, \rho_2 \in [0,1), \delta = 10^{-8}$

s=0, r=0 (moments 1 and 2), t=0

while stop criterion not met

randomly select m examples & labels (x, y)

estimate gradient $\hat{g} = \frac{1}{m} \nabla_\theta \sum_i L(f(x^{(i)} \mid \theta), y^{(i)})$

biased estimators

$$s = \rho_1 r + (1-\rho_1)\hat{g} \qquad \hat{E}[g]$$

$$r = \rho_2 r + (1-\rho_2)\hat{g} \odot \hat{g} \qquad \hat{E}[g^2]$$

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Adam

(continuation of while loop)

$t = t + 1$

correct for biases $\hat{s} = \frac{s}{1-\rho_1^t}$ $\hat{E}[g]$

$\hat{r} = \frac{r}{1-\rho_2^t}$ $\hat{E}[g^2]$

update model

similar to SGD w/momentum

$$\theta = \theta - \epsilon \frac{\hat{s}}{\sqrt{\delta + \hat{r}}}$$ element-wise operations

similar to RMSprop

Optimizers

- All the optimizers we have looked at are *first order* optimizers.
- No single algorithm has been shown to be the best

Second order optimizers

- Use the Hessian (or an approximation)
- We will not cover these in detail, but two examples covered in text
  - Newton's method – uses 2^{nd} order Taylor expansion
  - Conjugate gradient descent – when gradient direction changes, pick a direction that does not undo the progress along the gradient