Loss functions and Optimization

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Outline

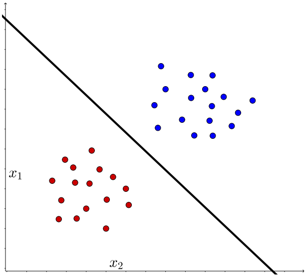
Loss Functions

Optimization

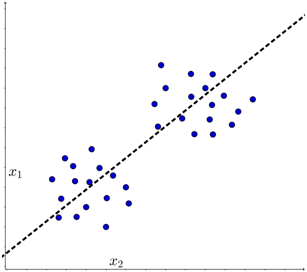
Loss Functions

Regression vs. classification

- **Classification:** Estimate a discrete variable for every input.
- **Regression:** Estimate a continuous variable for every input.



Classification



Regression

Loss function vs. last activation function in a network

The last activation function

- is applied on **individual samples** x_m **of the batch**
- is present at training **and testing**
- produces the output, or prediction
- generally produces a vector

The loss function

- combines **all** M **samples and labels**
- is **only** present at **training**
- produces the loss
- generally produces a scalar

Maximum Likelihood Estimation Reminder

Assume a

- Training set with
  - Observations: $\mathbf{X} = \mathbf{x}_1, \cdots, \mathbf{x}_M$
  - and associated labels $\mathbf{Y} = \mathbf{y}_1, \cdots, \mathbf{y}_M$
- and a model for a conditional probability density function $p\big(\mathbf{y}\big|\mathbf{x}\big)$

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Dataset

- Probability to observe $\mathbf{y}_m$ given observation $\mathbf{x}_m$ is $p(\mathbf{y}_m|\mathbf{x}_m)$
- Joint probability is $p(\mathbf{y}_m|\mathbf{x}_m) \cdot p(\mathbf{y}_i|\mathbf{x}_i)$ if they are:
  - **I**ndependent
  - and **I**dentically **D**istributed
- probability to observe $\mathbf{Y}$ is $\prod_{m=1}^{M} p(\mathbf{y}_m|\mathbf{x}_m)$

Likelihood function

- p governed by parameters $\mathbf{w}$

$$\underset{\mathbf{w}}{\text{maximize}} \quad \left\{ \prod_{m=1}^{M} p(\mathbf{y}_m | \mathbf{x}_m, \mathbf{w}) \right\}$$

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Negative Log Likelihood

- Maximum not affected by a monotonous transformation
- Maximization to minimization by flipping the sign
- $\underset{\mathbf{w}}{\text{minimize}} \quad \left\{ -\ln\left(L(\mathbf{w})\right) \right\} = \underset{\mathbf{w}}{\text{minimize}} \quad \left\{ \sum_{m=1}^{M} -\ln\left(p(\mathbf{y}_m | \mathbf{x}_m, \mathbf{w})\right) \right\}$

Regression

Assume a **univariate** Gaussian model:

$$p(y|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}\left(\hat{y}(\mathbf{x}, \mathbf{w}), \quad \frac{1}{\beta} \quad \right)$$

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$$= \frac{\sqrt{\beta}}{\sqrt{2\pi}} e^{\beta \frac{-(y_m - \hat{y}(\mathbf{x}_m, \mathbf{w}))^2}{2}}$$

Log Likelihood Function Regression

$$-\ln\left(L(\mathbf{w})\right) = \sum_{m=1}^{M} -\ln\left(\frac{\sqrt{\beta}}{\sqrt{2\pi}} e^{\beta\frac{-(y_m-\hat{y}(\mathbf{x}_m,\mathbf{w}))^2}{2}}\right)$$

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This can be generalized to vectors $\mathbf{y}_m, \hat{\mathbf{y}}$:

$$\frac{1}{2}\sum_{m=1}^{M}\|\mathbf{y}_m - \hat{\mathbf{y}}(\mathbf{x}_m, \mathbf{w})\|_2^2$$

Classification using an *L*-norm

L_2-loss and L_1-loss can be applied for classification

- They correspond to variants of minimizing the **expected misclassification probability**
- They cause **slow convergence** because they don't penalize heavily misclassified probabilities
- They might be advantageous in situations with **extreme label noise**

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Multi-class generalization: Multinoulli (Categorical, $\mathfrak{C}$) distribution

- $\mathbf{y}$, which is one-hot encoded

$$\mathfrak{C}(\mathbf{y}|\mathbf{p}) = \begin{cases} \prod_{k=0}^{K} p_k^{y_k} & \text{if } y_k \in \{0,1\} \\ 0 & \text{otherwise} \end{cases}$$

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- So the probability to observe $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ which is tail for this unfair coin is 70%.

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$$= -\sum_{m=1}^{M} \ln(\hat{y}_k(\mathbf{x}_m,\mathbf{w}))\big|_{y_{k,m}=1}$$

Relation to the Kullback Leibler Divergence

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We know that our ML estimation for a single sample has the form of cross-entropy:

$$-\sum_{k=0}^{K} \ln\left(\hat{y}_k^{y_k}\right) = \mathrm{H}(\mathbf{y}, \hat{\mathbf{y}})$$

and therefore is equal to minimizing the KL-divergence.

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- Of course. We just have to make sure $\hat{y}_k \in [0, 1] \, \forall k$
- This can be achieved using a sigmoid activation function
- **y** is simply no longer one-hot encoded
- As we've seen before this is equivalent to minimizing KL-divergence

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- L_2-loss can be used for **regression**
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- L_2-loss can be used for **regression**
- Cross-entropy-loss can be used for **classification**
- L_2-loss and Cross-entropy-loss can be derived as **ML-Estimators** from **strict** probabilistic assumptions
- In absence of more domain knowledge they are your **first choices**
- They are both intrinsically **multi-variate**

NEXT TIME

ON DEEP LEARNING

Loss functions and Optimization - Part 2

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Back to the Perceptron - again!

How does the Perceptron criterion fit into this?

$$\text{minimize} \quad \left\{ L(\mathbf{w}) = -\sum_{\mathbf{x}_m \in \mathcal{M}} y_m \cdot (\mathbf{w}^\mathsf{T} \mathbf{x}_m) \right\}$$

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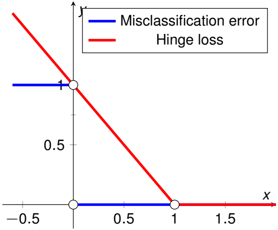
- ... and the gradient would vanish almost everywhere
- Sounds familiar?
- What did we do about that last time?

Hinge loss



$$L(\mathbf{w}) = \sum_{m=1}^{M} \max\left(0, 1 - y_m \hat{y}(\mathbf{x}_m, \mathbf{w})\right)$$

- Classification depends only on the sign
- If the signs match we get a positive value and classify correct
- Hinge loss is a convex approximation to the misclassification loss
- But what about the gradient?

Subgradients

Suppose we have a convex, differentiable function. Then we have:

$$f(\mathbf{x}) \geq f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T(\mathbf{x} - \mathbf{x}_0) \quad \forall \mathbf{x} \in \mathcal{X}$$

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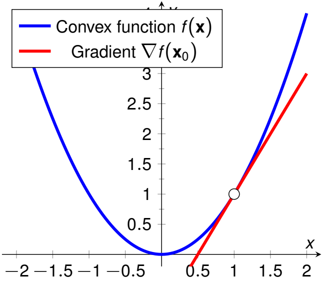

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- If f is differentiable at $\mathbf{x}_0$:

$$\partial f(\mathbf{x}_0) = \{\nabla f(\mathbf{x}_0)\}$$

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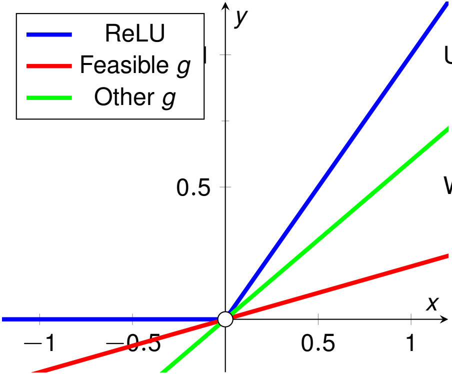

Using:

$$f(\mathbf{x}) \geq f(\mathbf{x}_0) + \mathbf{g}^T(\mathbf{x} - \mathbf{x}_0) \quad \forall \mathbf{x} \in \mathcal{X}$$

We get:

$$\partial f(x_0) = \begin{cases} 1 & \text{if } x_0 > 0 \\ 0 & \text{if } x_0 < 0 \\ g \in [0, 1] & \text{if } x_0 = 0 \end{cases}$$

- We already used this for the ReLU!
- Gradient descent was implicitly generalized to the subgradient algorithm

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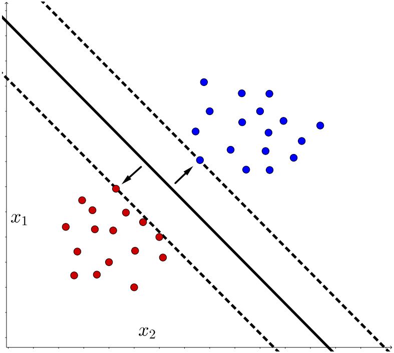
- Subgradients are a generalization of gradients for **convex, non-smooth functions**
- The gradient descent algorithm is replaced by the subgradient algorithm for these functions
- For piecewise continuous functions you just choose a particular subgradient and don’t even notice a difference
- This is basically just the solid math why this works
- We use this for the ReLU and Hinge loss so far

Isn't an SVM far more desirable?

SVM reminder



$$\min \quad \frac{1}{2}\|\mathbf{w}\|_2^2$$

$$s.t. \quad \forall m : -\left(y_m \cdot (\mathbf{w}^T \mathbf{x}_m) - 1 \qquad \right) \leq 0$$

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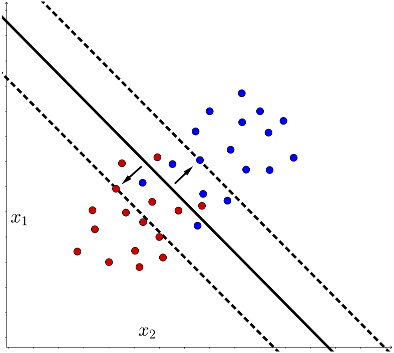

$$\min \quad \frac{1}{2}\|\mathbf{w}\|_2^2 + \gamma \sum_m \xi_m$$

$$s.t. \quad \forall m : -(y_m \cdot (\mathbf{w}^T \mathbf{x}_m) - 1 + \xi_m) \leq 0$$

$$\forall m : -\xi_m \leq 0$$

Isn't an SVM far more desirable?

- We construct the Lagrangian dual function

$$L(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_2^2 + \gamma \sum_{m=1}^{M} \xi_m + \sum_{m=1}^{M} \lambda_m(-y_m \cdot (\mathbf{w}^T \mathbf{x}_m) + 1 - \xi_m) - \sum_{m=1}^{M} \nu_m \xi_m$$

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&= \frac{1}{2}\|\mathbf{w}\|_2^2 + \sum_{m=1}^{M} (\gamma \xi_m - \nu_m \xi_m - \lambda_m \xi_m) + \sum_{m=1}^{M} \lambda_m (1 - y_m \cdot (\mathbf{w}^T \mathbf{x}_m))
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&\approx \frac{1}{2} \quad \|\mathbf{w}\|_2^2 \quad + \gamma \sum_{m=1}^{M} \max(0, 1 - y_m \cdot (\mathbf{w}^T \mathbf{x}_m))
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Isn't an SVM far more desirable?

- We construct the Lagrangian dual function
- Remember: $\lambda_m \geq 0$
- Equivalent "up to an overall multiplicative constant"[1]

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L(\mathbf{w}) &= \frac{1}{2}\|\mathbf{w}\|_2^2 + \gamma \sum_{m=1}^{M} \xi_m + \sum_{m=1}^{M} \lambda_m(-y_m \cdot (\mathbf{w}^T \mathbf{x}_m) + 1 - \xi_m) - \sum_{m=1}^{M} \nu_m \xi_m \\
&= \frac{1}{2}\|\mathbf{w}\|_2^2 + \sum_{m=1}^{M} (\gamma \xi_m - \nu_m \xi_m - \lambda_m \xi_m) + \sum_{m=1}^{M} \lambda_m (1 - y_m \cdot (\mathbf{w}^T \mathbf{x}_m)) \\
&\approx \frac{1}{2} \underbrace{\|\mathbf{w}\|_2^2}_{L2 \text{ regularizer}} + \gamma \sum_{m=1}^{M} \underbrace{\max(0, 1 - y_m \cdot (\mathbf{w}^T \mathbf{x}_m))}_{\text{Hinge loss}}
\end{aligned}
$$

Open points

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Outliers are punished linearly

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- A variant of the hinge loss which penalizes outliers more strongly [4]:

$$L(\mathbf{w}) = \sum_{m=1}^{M} \left(\max\left(0, 1 - y_m \hat{y}(\mathbf{x}_m, \mathbf{w})\right)\right)^2$$

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How to apply SVMs to multi-class problems?

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How to apply SVMs to multi-class problems?

- A Hinge loss for multi-class problems [9]:

$$L(\mathbf{w}) = \sum_{m=1}^{M} \sum_{k \neq c}^{K} \max\left(0, 1 - \hat{y}_c(\mathbf{x}_m, \mathbf{w}) + \hat{y}_k(\mathbf{x}_m, \mathbf{w})\right)$$

Summary

- We have seen we can incorporate an SVM into a neural network
- See [4] for a reference using this
- We've learned before how to deal with the non-smooth objective

NEXT TIME

ON DEEP LEARNING

Loss functions and Optimization - Part 3

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Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
April 24, 2023

Optimization

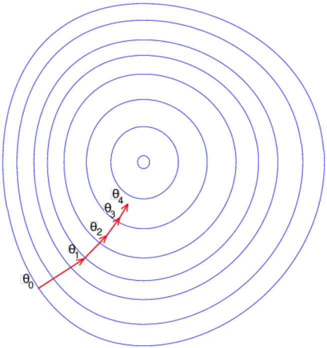
Gradient Descent revisited

Goal: Optimize empirical risk:

$$\mathbb{E}_{\mathbf{x},\mathbf{y}\sim\hat{p}_{\text{data}}(\mathbf{x},\mathbf{y})}\left[L(\mathbf{w},\mathbf{x}_m,\mathbf{y}_m)\right] = \frac{1}{M}\sum_{m=1}^{M} L(\mathbf{w},\mathbf{x},\mathbf{y})$$

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta\nabla L(\mathbf{w}^{(k)},\mathbf{x},\mathbf{y})$$

- Step size defined by learning rate η
- Gradient with respect to **every** sample
- Guaranteed to converge to a **local minimum**



Rethinking Gradient Descent

For each iteration...

- Batch Gradient Descent: Use all M samples

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  - Small batches offer regularization effect ➔ need smaller η
  - Regains efficiency ➔ the standard case in deep learning

How can this even work?

- Optimization problem is non-convex
- Exponential number of local minima

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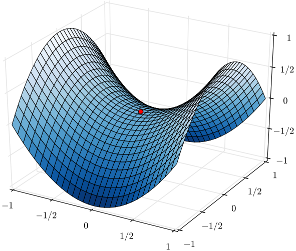
- Exponential number of local minima

Possible Answers (Choromanska et al. 2015, Dauphin et al. 2014)

- High dimensional function
- Local minima exist but very close to global minima
- ... and many of those are equivalent

→ Presumably more critical: saddle points

- Local minimum might be better than global minima (overfitting!)



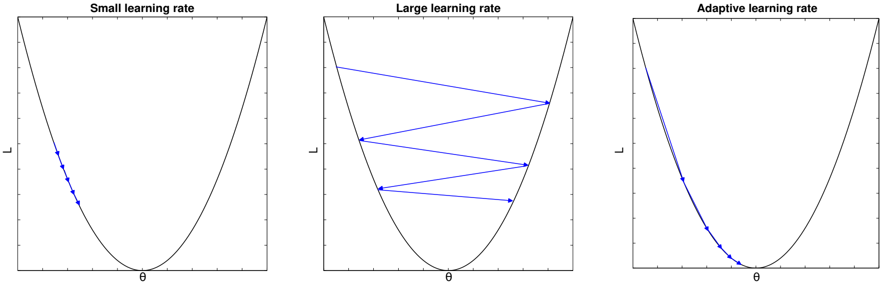
Source: https://upload.wikimedia.org/wikipedia/commons/1/1e/Saddle_point.svg

Another possible answer

Possible answer (Percy Liang, NIPS 2016)

- “overprovisioning”
- Many different ways how a network can approximate the desired relationship
- Only needs to find one
- This has been verified experimentally by learning **random** labels [10]

SGD – Learning Rate Choice



- η too small: long training time
- η too large: miss optima
- Practice: "learning rate decay": adapt η gradually (e.g.: start with $\eta = 0.01$ and divide every *x* epoch by 10)

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- L-BFGS doesn't perform well outside of batch settings
- A report on this was presented by Google [7]

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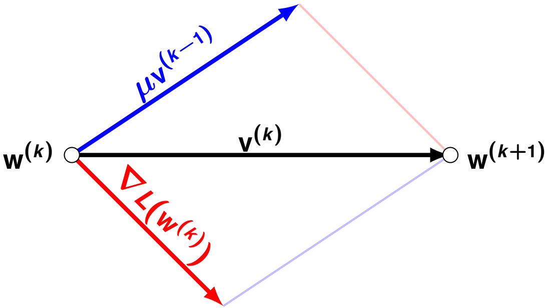

Momentum

- Parameter update based on current and past gradients:

$$\mathbf{v}^{(k)} = \underbrace{\mu}_{\text{momentum}} \mathbf{v}^{(k-1)} - \eta \nabla L(\mathbf{w}^{(k)})$$

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− Still learning rate decay needed!

Nesterov Accelerated Gradient (NAG) / Nesterov Momentum

- "Look ahead" - compute the gradient in the direction we're going anyway!

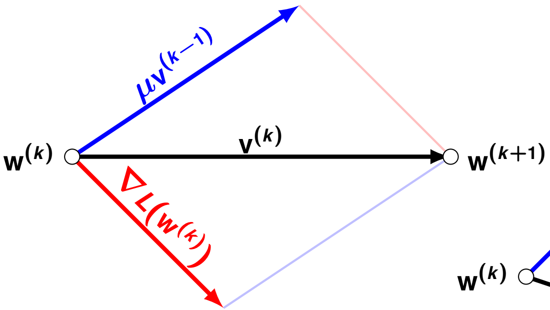
$$\mathbf{v}^{(k)} = \mu \mathbf{v}^{(k-1)} - \eta \nabla L(\underbrace{\mathbf{w}^{(k)} + \mu \mathbf{v}^{(k-1)}}_{\text{approx. of next parameters}})$$

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} + \mathbf{v}^{(k)}$$

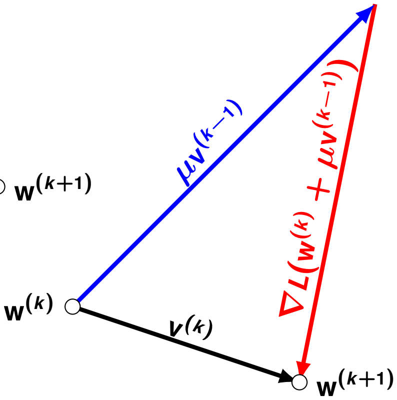
- We can rewrite this to use the conventional gradient:

$$\mathbf{v}^{(k)} = \mu \mathbf{v}^{(k-1)} - \eta \nabla L(\mathbf{w}^{(k)})$$
$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \mu \mathbf{v}^{(k-1)} + (1+\mu)\mathbf{v}^{(k)}$$

How does this compare to momentum?

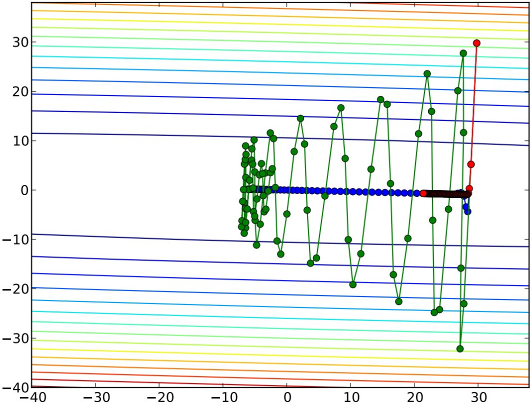


Momentum



Nesterov Momentum

Example for an advantage of NAG



GD (red), momentum (green), NAG (blue)

Source: Sutskever “Training Recurrent Neural Networks”, p. 76

What if our features have different needs?

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- Suppose some features are activated very infrequently
- ... while others are updated very often

What if our features have different needs?

- Suppose some features are activated very infrequently
- ... while others are updated very often
- We'd need individual learning rates for every parameter in the network
- Large (small) learning rates for infrequent (frequent) parameters and parameters with small (large) gradient magnitudes

AdaGrad

$$\mathbf{g}^{(k)} = \nabla L(\mathbf{w}^{(k)})$$

$$\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} + \mathbf{g}^{(k)} \odot \mathbf{g}^{(k)}$$

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \frac{\eta}{\sqrt{\mathbf{r}^{(k)}} + \epsilon} \odot \mathbf{g}^{(k)}$$

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- **Ada**ptive **Grad**ient
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\+ Individual learning rates

− Learning rate decreases too aggressively

RMSProp

$$
\begin{aligned}
\mathbf{g}^{(k)} &= \nabla L(\mathbf{w}^{(k)}) \\
\mathbf{r}^{(k)} &= \rho \mathbf{r}^{(k-1)} + (1-\rho)\mathbf{g}^{(k)} \odot \mathbf{g}^{(k)} \\
\mathbf{w}^{(k+1)} &= \mathbf{w}^{(k)} - \frac{\eta}{\sqrt{\mathbf{r}^{(k)}} + \epsilon} \odot \mathbf{g}^{(k)}
\end{aligned}
$$

- Hinton suggests $\rho = 0.9$, $\eta = 0.001$

\+ The aggressive decrease is fixed

− We still have to set the learning rate

Adadelta

$$
\begin{aligned}
\mathbf{g}^{(k)} &= \nabla L(\mathbf{w}^{(k)}) \\
\mathbf{r}^{(k)} &= \rho \mathbf{r}^{(k-1)} + (1-\rho)\mathbf{g}^{(k)} \odot \mathbf{g}^{(k)} \\
\boldsymbol{\Delta}_x &= -\frac{\sqrt{\mathbf{h}^{(k-1)}}}{\sqrt{\mathbf{r}^{(k)}} + \epsilon} \odot \mathbf{g}^{(k)} \\
\mathbf{h}^{(k)} &= \rho \mathbf{h}^{(k-1)} + (1-\rho)\boldsymbol{\Delta}_x \odot \boldsymbol{\Delta}_x \\
\mathbf{w}^{(k+1)} &= \mathbf{w}^{(k)} + \boldsymbol{\Delta}_x
\end{aligned}
$$

- Suggested: $\rho = 0.95$

\+ No learning rate

Adam

$$\mathbf{g}^{(k)} = \nabla L(\mathbf{w}^{(k)})$$

$$\mathbf{v}^{(k)} = \mu \mathbf{v}^{(k-1)} + (1-\mu)\mathbf{g}^{(k)}$$

$$\mathbf{r}^{(k)} = \rho \mathbf{r}^{(k-1)} + (1-\rho)\mathbf{g}^{(k)} \odot \mathbf{g}^{(k)}$$

$$\text{Bias correction: } \hat{\mathbf{v}}^{(k)} = \frac{\mathbf{v}^{(k)}}{1-\mu^k} \quad \hat{\mathbf{r}}^{(k)} = \frac{\mathbf{r}^{(k)}}{1-\rho^k}$$

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \frac{\hat{\mathbf{v}}^{(k)}}{\sqrt{\hat{\mathbf{r}}^{(k)}} + \epsilon}$$

- Short for **Ada**ptive **M**oment Estimation
- Suggested: $\mu = 0.9, \rho = 0.999, \eta = 0.001$
- \+ Robustness
- Combination w. NAG exists (“Nadam”)

AMSGrad

- Adam empirically observed to fail to converge to an optimal/good solution

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- Recent insight by Reddi et al. [5]: Adam (and similar methods) **do not guarantee** convergence for convex problems (error in original convergence proof)
- AMSGrad [5] “fixes” Adam to ensure non-increasing step size:

$$\hat{\mathbf{v}}^{(k)} = \max(\hat{\mathbf{v}}^{(k-1)}, \mathbf{v}^{(k)})$$

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- Effect has to be shown in larger experiments
- Lesson: Keep your eyes open!

Summary

- SGD + Nesterov momentum + learning rate decay
  - \+ Often converges most reliably
  - \+ Still used in many state-of-the-art papers
  - − Learning rate decay needs to be adjusted
- Adam
  - \+ Individual learning rates
  - \+ Learning rate very well behaved
  - − Loss curves harder to interpret
- **Not discussed**: Distributed gradient descend

Practical recommendations

- Start by using minibatch SGD with momentum
- Mostly keep to the default momentum
- Give Adam a try when you have a feeling for your data
- When in need for individual learning rates use Adam
- Start by using the default parameters for Adam
- Adjust the learning rate first
- Keep your eyes open for unusual behavior (see AMSGrad)

NEXT TIME

ON DEEP LEARNING

Coming Up

- How can we deal with spatial correlation in features?
- Why do we hear so much about convolution in neural networks?
- How can we incorporate invariances into network architectures?

Comprehensive Questions

- What are our standard loss functions for classification and regression?
- What assumptions do our standard loss functions imply?
- What is a subdifferential at a point $\mathbf{x}_0$?
- How can we optimize a non-smooth convex function?
- What if somebody tells you, to use an SVM because it is superior?
- What is Nesterov Momentum?
- Describe Adam.

Further Reading

- Link - for details on Maximum Likelihood estimation and the basic loss functions.
- Link - [6] for insights about some loss functions
- Link - [10] for a troubling insight, that deep networks can learn arbitrary random labels

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