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SCHOOL OF ENGINEERING

Loss functions and Optimization

A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle, K. Packhäuser, M. Zinnen

Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg

April 24, 2023

Outline

Loss Functions

Optimization

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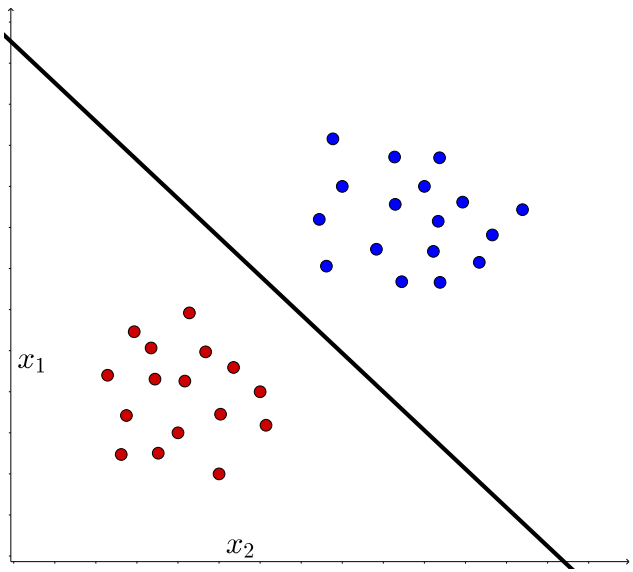
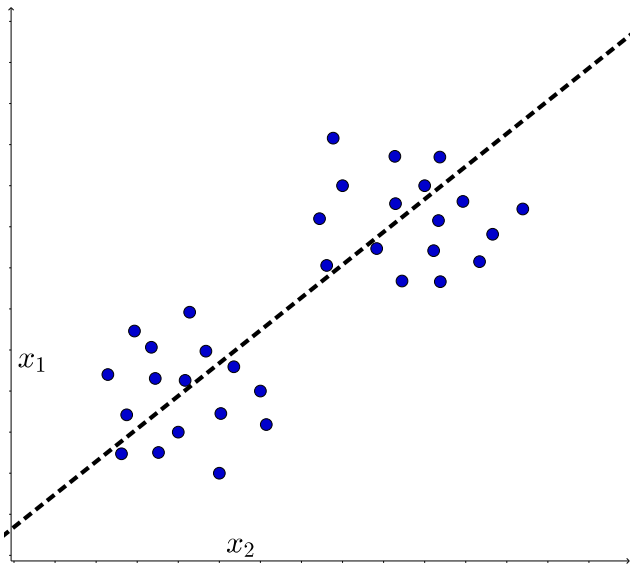
Loss Functions

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 $p(\mathbf{y}|\mathbf{x})$

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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
- $\underset{\mathbf{w}}{\text{minimize}} \quad \{ -\ln(L(\mathbf{w})) \} = \underset{\mathbf{w}}{\text{minimize}} \quad \{ \sum_{m=1}^{M} -\ln(p(\mathbf{y}_m | \mathbf{x}_m, \mathbf{w})) \}$

Regression

Assume a **univariate** Gaussian model:

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

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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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When optimizing for $\mathbf{w}$ - eliminate constants and factors:

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

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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- We encode head as $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and tail as $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$
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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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$$= -\sum_{m=1}^{M} \ln(\hat{y}_k(\mathbf{x}_m,\mathbf{w}))|_{y_{k,m}=1}$$

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.

Can we also use cross-entropy for regression?

Can we also use cross-entropy for regression?

- 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

Summary

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- L_2-loss can be used for **regression**
- Cross-entropy-loss can be used for **classification**

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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

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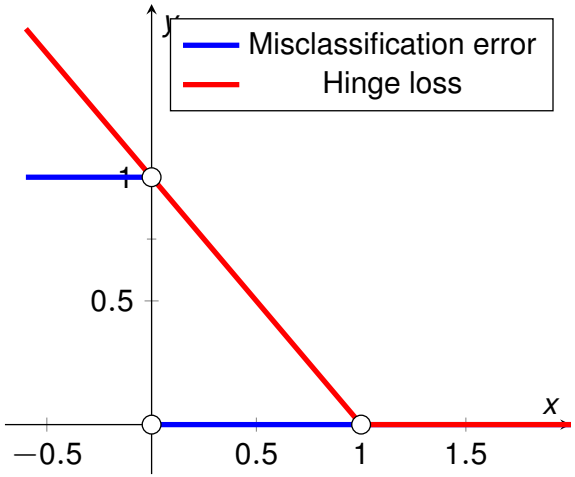
- ... and the gradient would vanish almost everywhere
- Sounds familiar?
- What did we do about that last time?

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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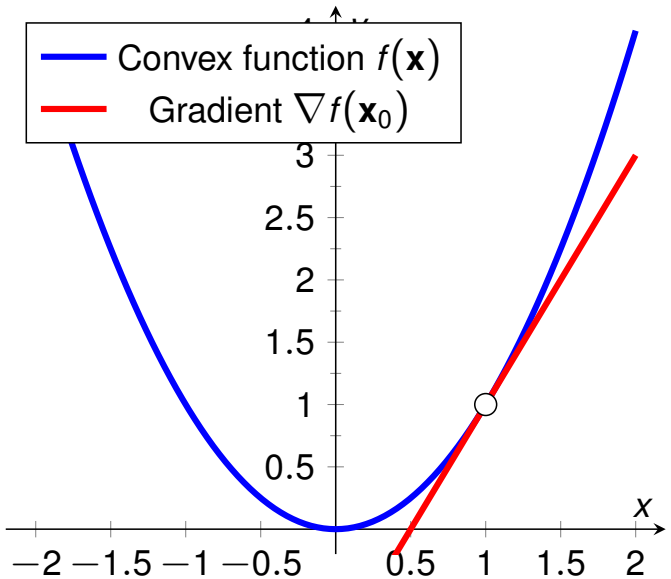

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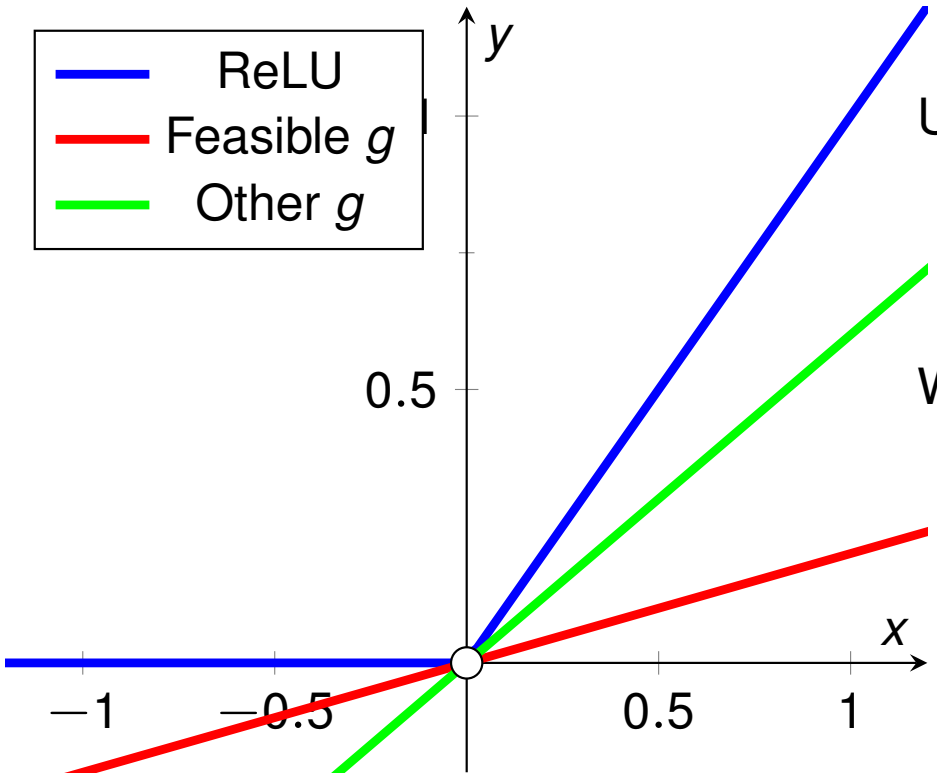
- If f is differentiable at $\mathbf{x}_0$:

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

Subgradients



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

Summary

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- The gradient descent algorithm is replaced by the subgradient algorithm for these functions

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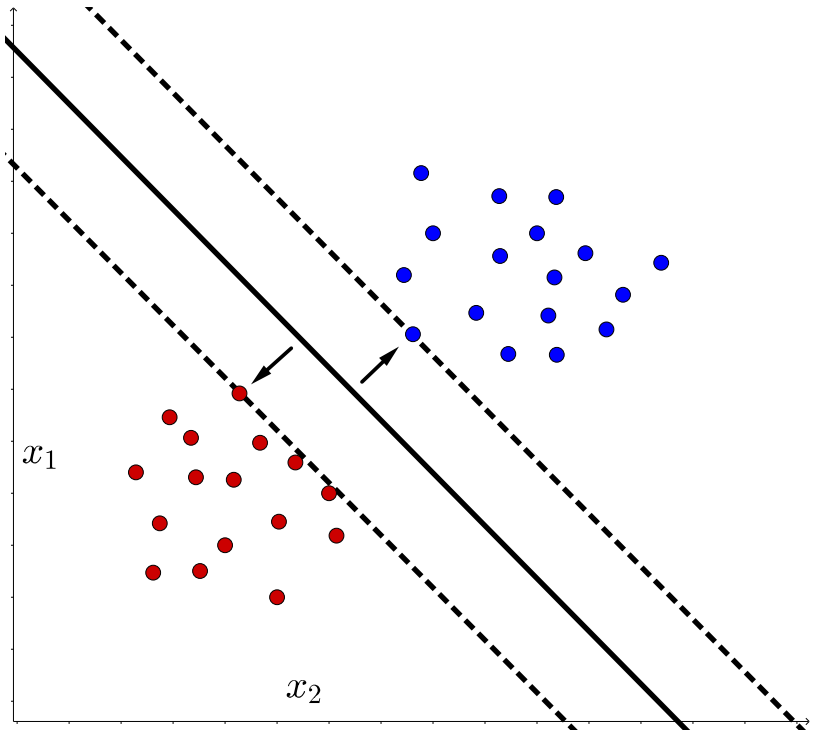
- Subgradients are a generalization of gradients for **convex, non-smooth functions**
- The gradient descent algorithm is replaced by the subgradient algorithm for these functions
- For piecewise continuous functions you just choose a particular subgradient and don't even notice a difference
- This is 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

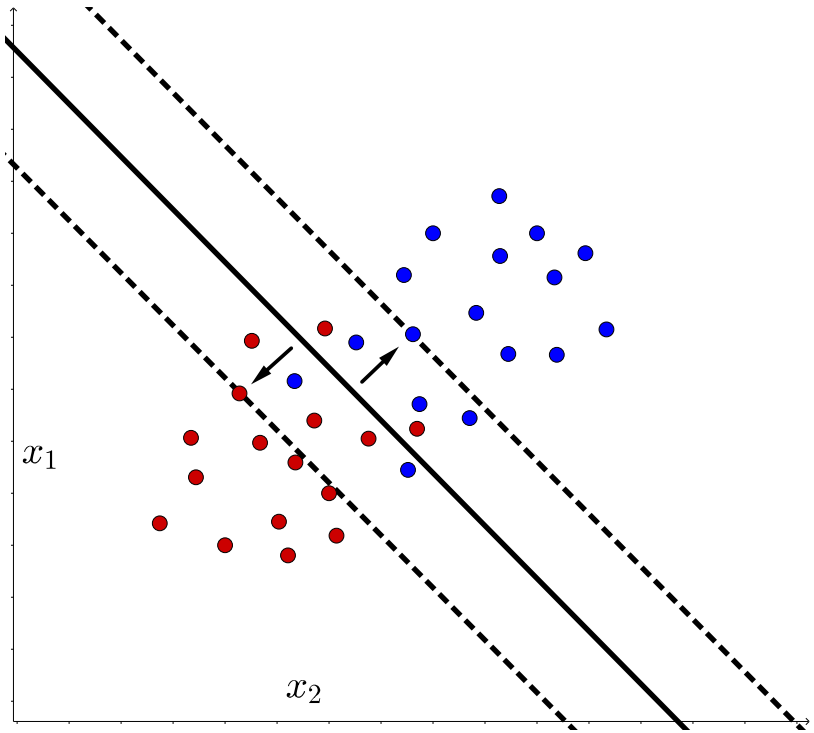


$$min \quad \frac{1}{2}\|\mathbf{w}\|_2^2$$

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

Isn't an SVM far more desirable?

SVM reminder



$$
\begin{aligned}
\textit{min} \quad & \frac{1}{2}\|\mathbf{w}\|_2^2 + \gamma \sum_m \xi_m \\
\textit{s.t.} \quad & \forall m : -\left(y_m \cdot \left(\mathbf{w}^T \mathbf{x}_m\right) - 1 + \xi_m\right) \leq 0 \\
& \forall m : -\xi_m \leq 0
\end{aligned}
$$

Isn't an SVM far more desirable?

- We construct the Lagrangian dual function

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

Isn't an SVM far more desirable?

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

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- Remember: $\lambda_m \geq 0$

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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))
\end{aligned}
$$

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]

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

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

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SCHOOL OF ENGINEERING

Loss functions and Optimization - Part 3

A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle, K. Packhäuser, M. Zinnen

Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg

April 24, 2023

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Optimization

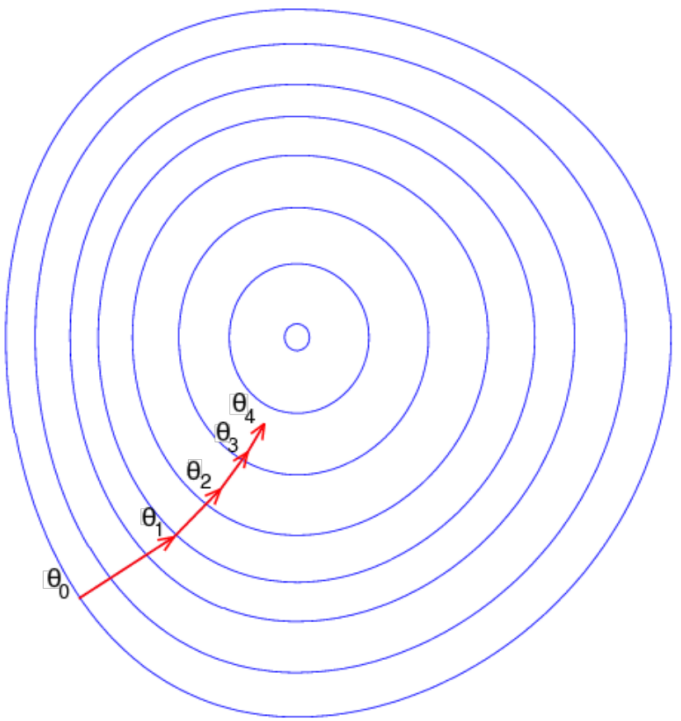
Gradient Descent revisited

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

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- Exponential number of local minima

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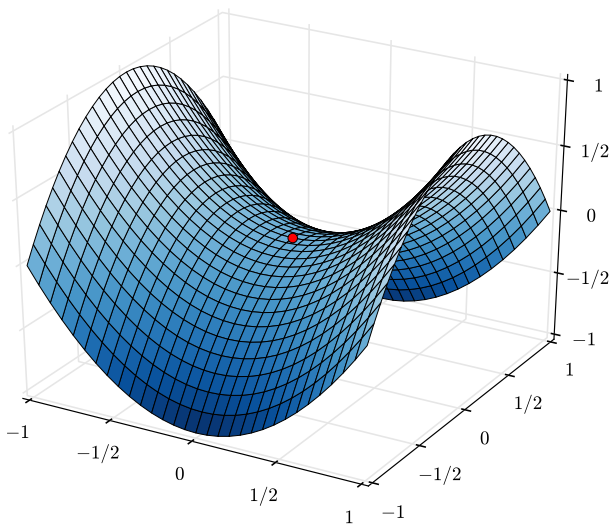
- Exponential number of local minima

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

$\rightarrow$ Presumably more critical: saddle points

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



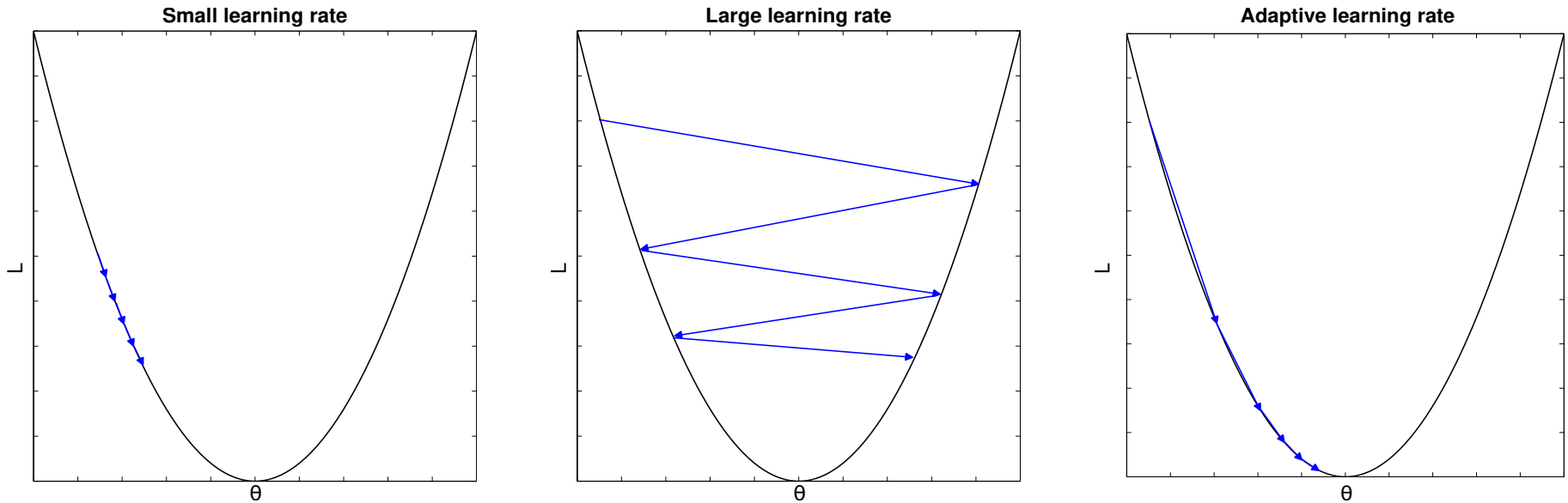
Source: https://upload.wikimedia.org/wikipedia/commons/1/1e/Saddle_point.svg

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)

Can't we get rid of this magic η?

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- The Hessian matrix $H\left(L(\mathbf{w}^{(k)})\right)$ is too expensive to calculate
- L-BFGS doesn't perform well outside of batch settings
- A report on this was presented by Google [7]

What can we do?

Idea: Accelerate in directions with persistent gradients

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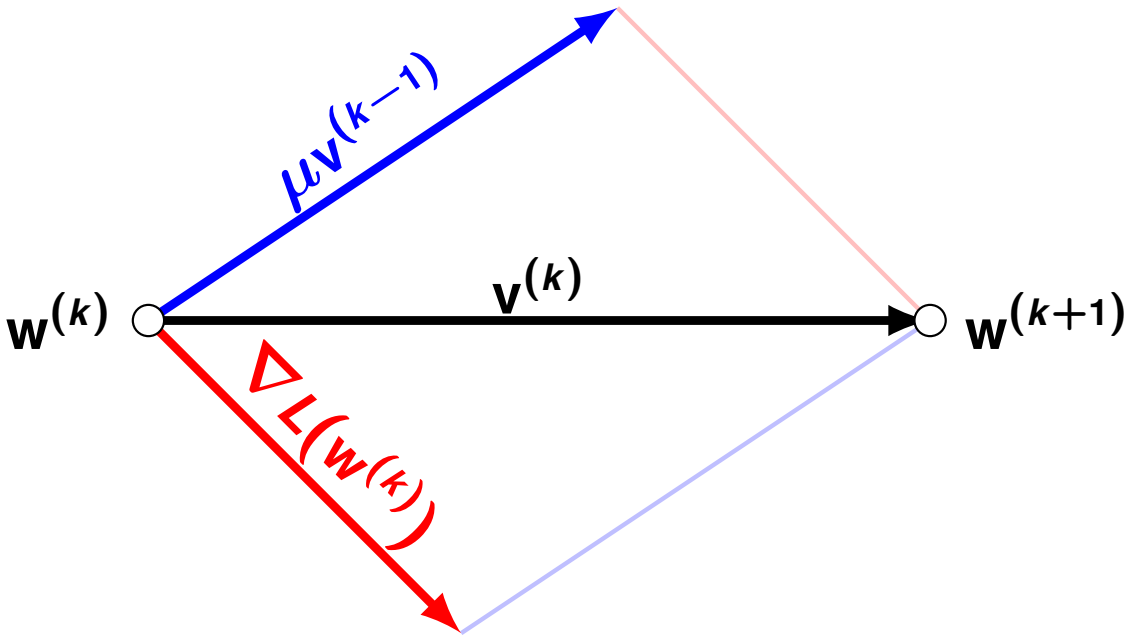

Momentum

- 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!

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

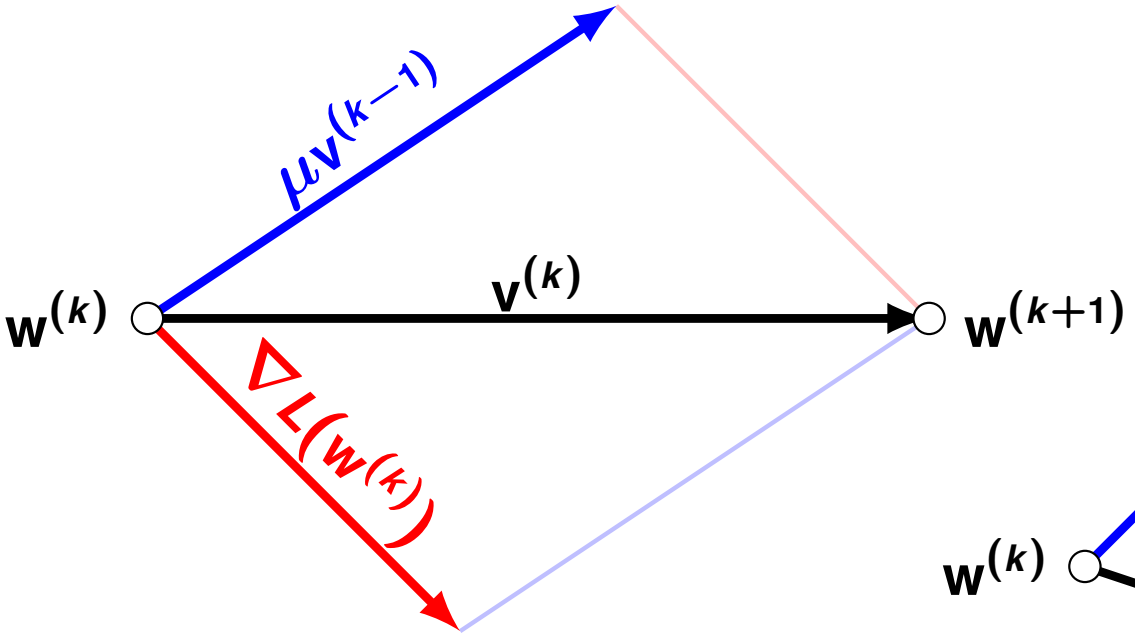
$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} + \mathbf{v}^{(k)}$$

- 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?



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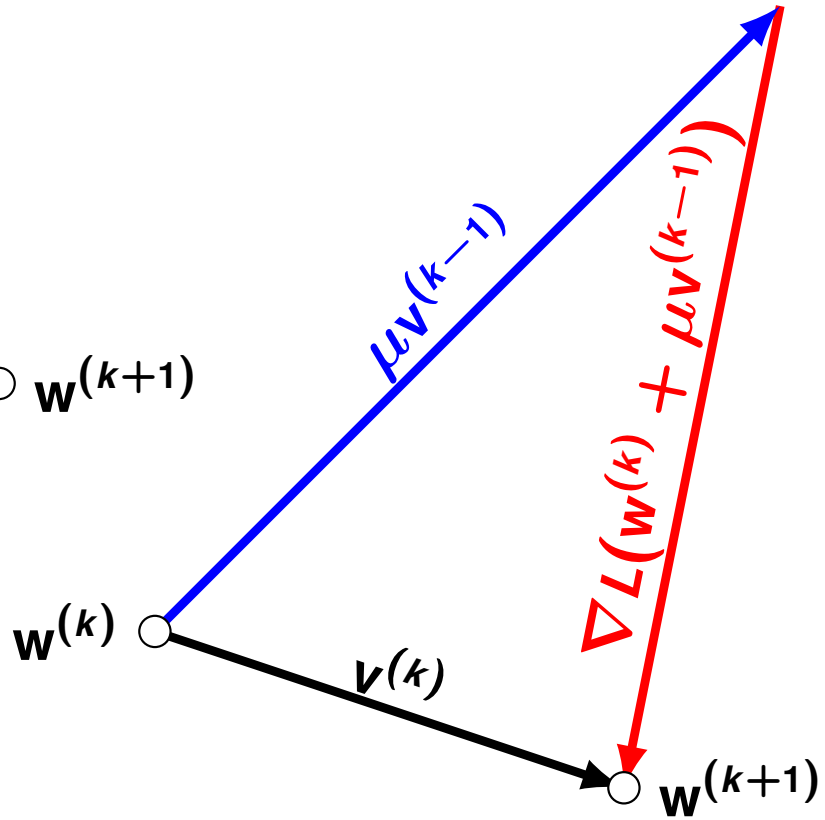
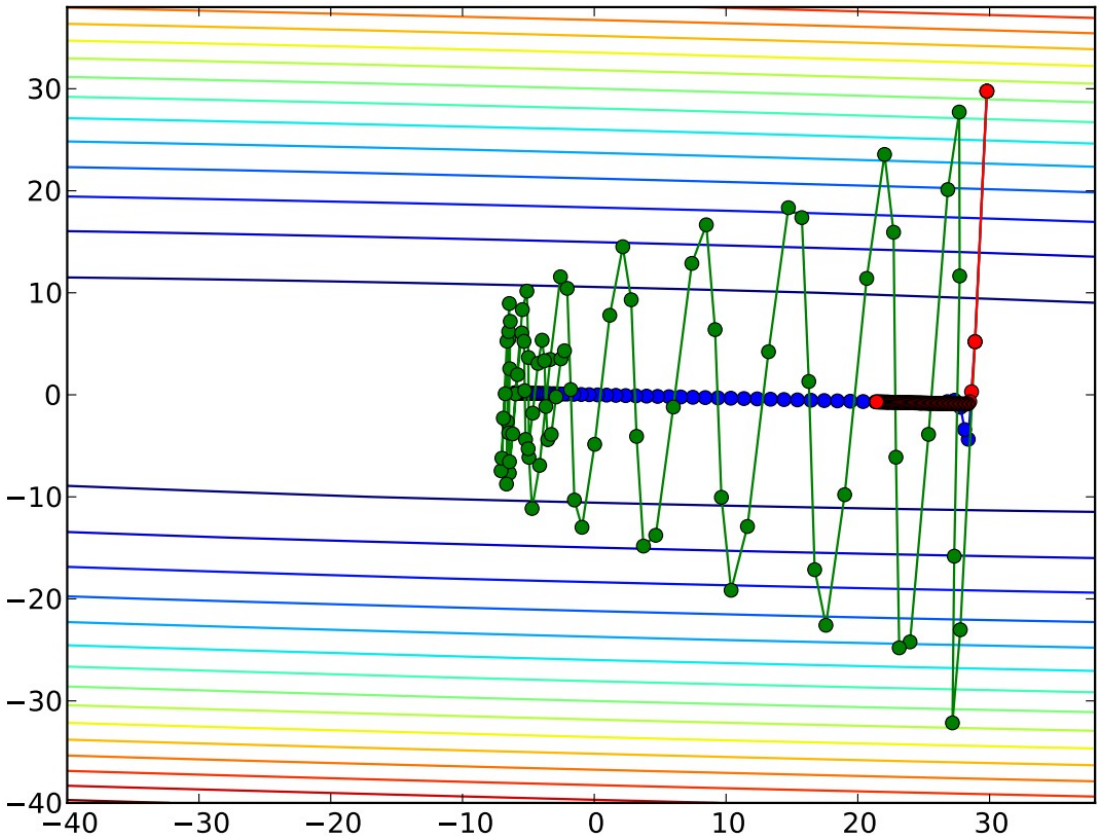


Nesterov Momentum

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

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

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

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

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

\− Learning rate decreases too aggressively

RMSProp

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

- Hinton suggests $\rho = 0.9$, $\eta = 0.001$
- \+ The aggressive decrease is fixed
- – We still have to set the learning rate

Adadelta

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

- Suggested: $\rho = 0.95$

\+ No learning rate

Adam

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

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

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

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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- 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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