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Loss functions and Optimization

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Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
April 28, 2020





Outline

Loss Functions

Optimization



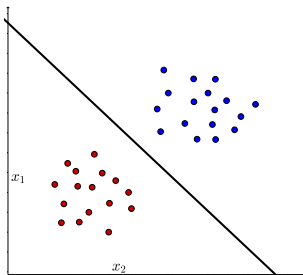
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Loss Functions

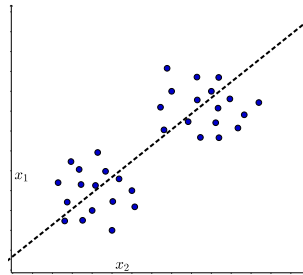


Regression vs. classification

- **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: $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_M$
 - and associated labels $\mathbf{Y} = \mathbf{y}_1, \dots, \mathbf{y}_M$
- 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:
 - Independent
 - and Identically Distributed
- 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

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

Regression

Assume a **univariate** Gaussian model:

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

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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

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

Log Likelihood Function Regression

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

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L^2 -loss

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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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Bernoulli distribution

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

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

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

Example for \mathfrak{C}

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- The probability of this is $\mathfrak{C}(\mathbf{y}|\mathbf{p}) = p_0^0 \cdot p_1^1 = 1 \cdot 0.7 = 0.7$
- So the probability to observe $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ which is tail for this unfair coin is 70%.

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Negative log Likelihood

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

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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

$$\text{KL}(p, q) = \int_{-\infty}^{+\infty} p(x) \ln \frac{p(x)}{q(x)} dx$$

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 \end{aligned}$$

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

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

and therefore is equal to minimizing the KL-divergence.

Can we also use cross-entropy for regression?

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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
- \mathbf{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?

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

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- ... and the gradient would vanish almost everywhere

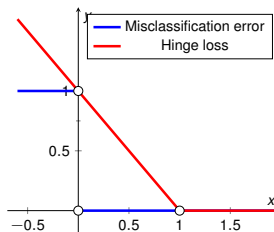
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- ... and the gradient would vanish almost everywhere
- Sounds familiar?
- What did we do about that last time?

Hinge loss



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

- 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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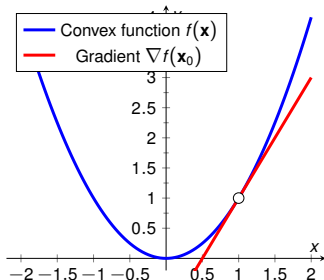
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In words: If we follow the gradient from any point of a convex function and check against the function, its value at the same \mathbf{x} will be higher.



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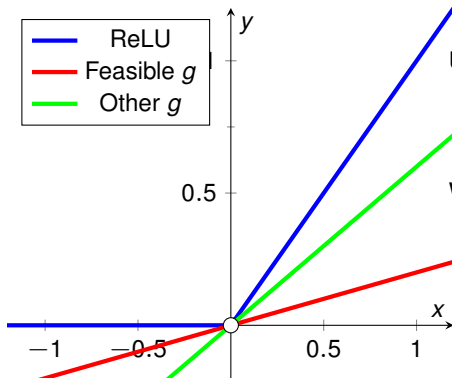
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$$\partial f(\mathbf{x}_0) := \{\mathbf{g}\}$$

- 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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- Subgradients are a generalization of gradients for **convex, non-smooth functions**
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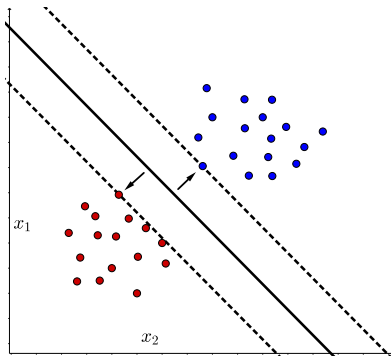
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- The gradient descent algorithm is replaced by the subgradient algorithm for these functions
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- This is basically just the solid math why this works
- We use this for the ReLU and Hinge loss so far

Isn't an SVM far more desirable?

SVM reminder

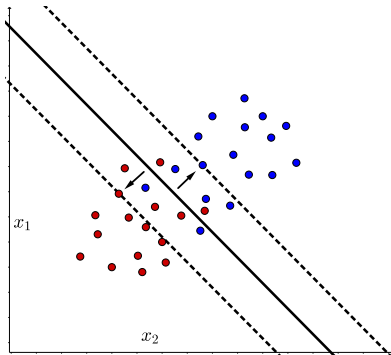


$$\min \quad \frac{1}{2} \|\mathbf{w}\|_2^2$$

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

Isn't an SVM far more desirable?

SVM reminder



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

Isn't an SVM far more desirable?

- We construct the Lagrangian dual function

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

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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]

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

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]:

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How to apply SVMs to multi-class problems?

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

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

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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Loss functions and Optimization - Part 3

A. Maier, V. Christlein, K. Breininger, S. Vesal, F. Meister, C. Liu, S. Gündel, S. Jaganathan, N. Maul, M. Vornehm, L. Reeb, F. Thamm, M. Hoffmann, C. Bergler, F. Denzinger, W. Fu, B. Geissler, Z. Yang
Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
April 28, 2020





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Optimization



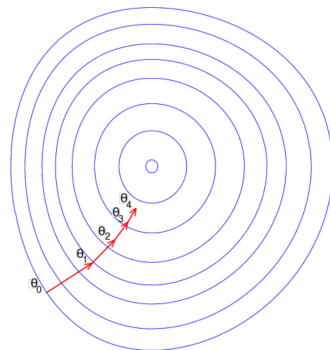
Gradient Descent revisited

Goal: Optimize empirical risk:

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

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

- 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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$$\mathbf{g}^{(k)} := \nabla L(\mathbf{w}^{(k)}) = \frac{1}{B} \nabla \sum_{b=1}^B L(\mathbf{w}^{(k)}, \mathbf{x}_b)$$

Rethinking Gradient Descent

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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?

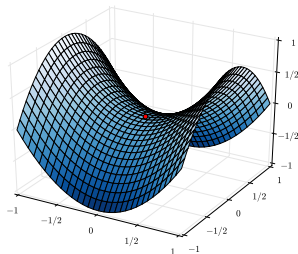
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How can this even work?

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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!)



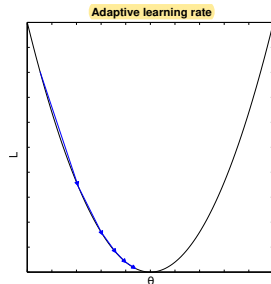
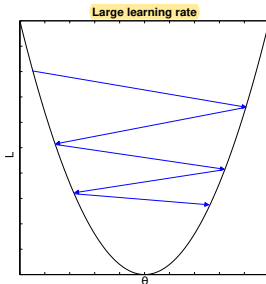
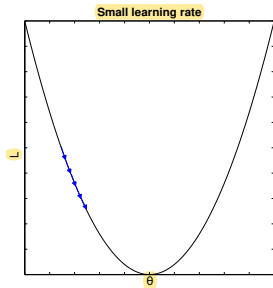
Source: https://upload.wikimedia.org/wikipedia/commons/1/1e/Saddle_point.svg

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)

Can't we get rid of this magic η ?

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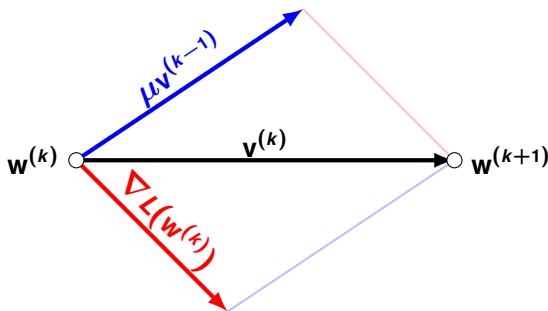
- The Hessian matrix $H\left(L(\mathbf{w}^{(k)})\right)$ is too expensive to calculate
- L-BFGS doesn't perform well outside of batch settings
- A report on this was presented by Google [7]

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!

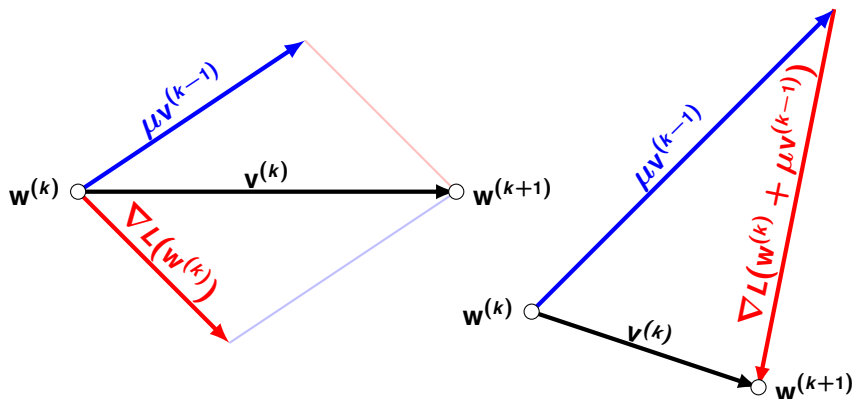
$$\mathbf{v}^{(k)} = \mu \mathbf{v}^{(k-1)} - \eta \nabla L(\underbrace{\mathbf{w}^{(k)} + \mu \mathbf{v}^{(k-1)}}_{\text{approx. of next parameters}})$$

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

- We can rewrite this to use the conventional gradient:

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

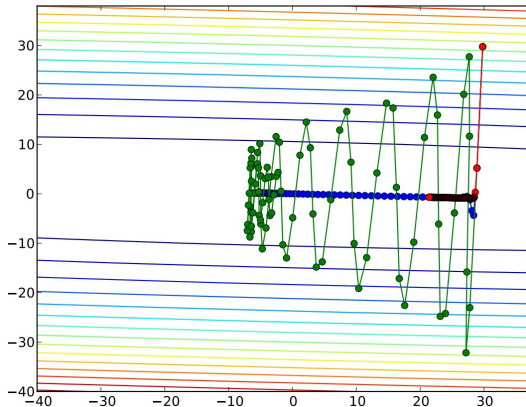
How does this compare to momentum?



Momentum

Nesterov Momentum

Example for an advantage of NAG



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

Source: Sutskever "Training Recurrent Neural Networks", p. 76

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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

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

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

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

- **Adaptive Gradient**
- Adaption based on all past squared gradients
- We use \odot to emphasize the element-wise multiplication

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- **Adaptive Gradient**
- Adaption based on all past squared gradients
- We use \odot to emphasize the element-wise multiplication
- + 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

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

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

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

$$\mathbf{h}^{(k)} = \rho \mathbf{h}^{(k-1)} + (1 - \rho) \Delta_x \odot \Delta_x$$

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

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

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

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

AMSGrad

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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)
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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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- [10] Chiyuan Zhang, Samy Bengio, Moritz Hardt, et al. "Understanding deep learning requires rethinking generalization". In: [arXiv preprint arXiv:1611.03530](#) (2016).