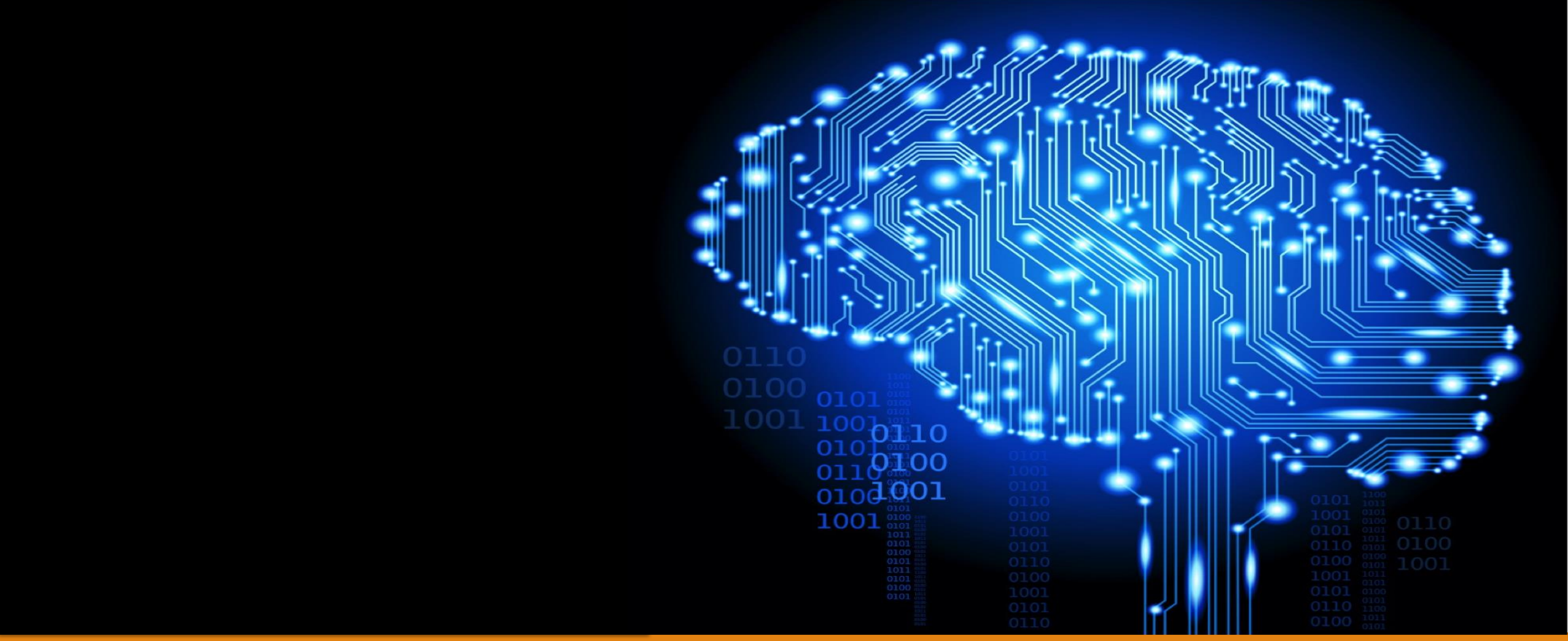

Lecture 3: Deeper into Deep Learning and Optimizations

Deep Learning @ UvA

Previous lecture

- Machine Learning Paradigm for Neural Networks
- The Backpropagation algorithm for learning with a neural network
- Neural Networks as modular architectures
- Various Neural Network modules
- How to implement and check your very own module

Lecture overview

- How to defining our model and optimize it in practice
- Data preprocessing and normalization
- Optimization methods
- Regularizations
- Architectures and architectural hyper-parameters
- Learning rate
- Weight initializations
- Good practices

Deeper into Neural Networks & Deep Neural Nets

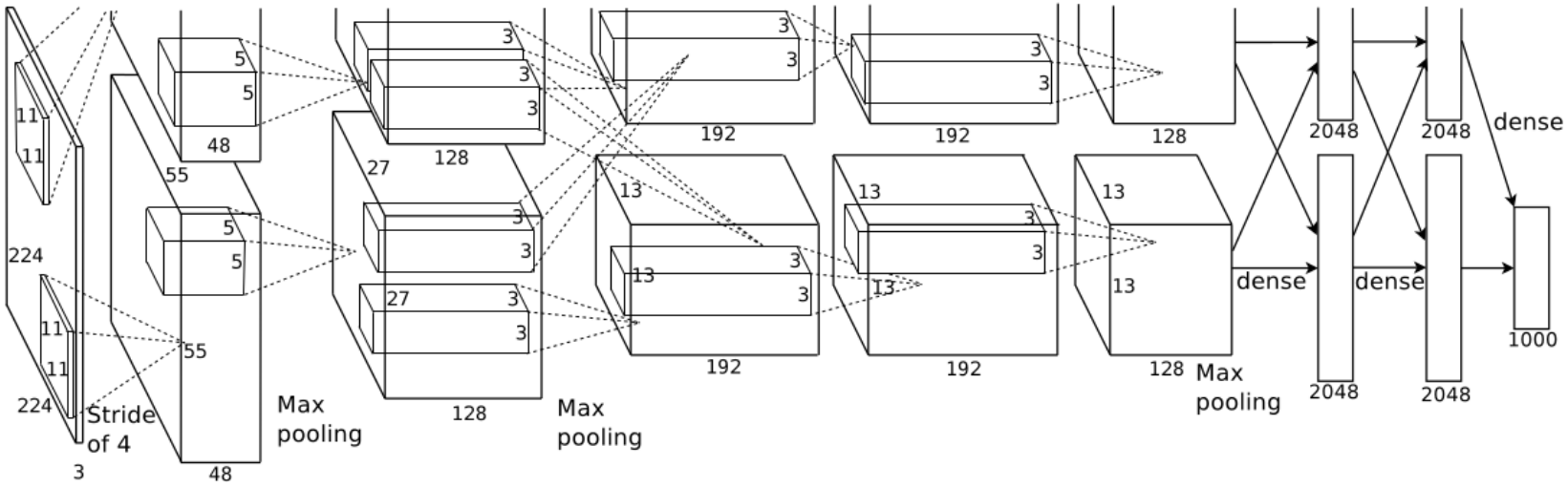

Figure 2: An illustration of the architecture of our CNN, explicitly showing the delineation of responsibilities between the two GPUs. One GPU runs the layer-parts at the top of the figure while the other runs the layer-parts at the bottom. The GPUs communicate only at certain layers. The network's input is 150,528-dimensional, and the number of neurons in the network's remaining layers is given by 253,440–186,624–64,896–64,896–43,264–4096–4096–1000.

A Neural/Deep Network in a nutshell

1. The Neural Network

$$a_L\left(x;\theta_{1,\ldots,\mathrm{L}}\right)=h_L\left(h_{L-1}(\ldots h_1(x,\theta_1),\theta_{L-1}),\theta_L\right)$$

2. Learning by minimizing empirical error

$$\theta^*\leftarrow\arg\min_\theta\sum_{(x,y)\subseteq(X,Y)}\mathcal{L}(y,a_L\left(x;\theta_{1,\ldots,\mathrm{L}}\right))$$

3. Optimizing with Gradient Descend based methods

$$\theta^{(t+1)}=\theta^{(t)}-\eta_t\nabla_\theta\mathcal{L}$$

SGD vs GD

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2. Learning by minimizing empirical error

$$\theta^* \leftarrow \arg\min_\theta \sum_{(x,y)\subseteq(X,Y)} \mathcal{L}\left(y, a_L\left(x;\theta_{1,\ldots,\mathrm{L}}\right)\right)$$

3. Optimizing with Gradient Descend based methods

$$\theta^{(t+1)} = \theta^{(t)} - \eta_t \nabla_\theta \mathcal{L}$$

Backpropagation again

- **Step 1.** Compute forward propagations for all layers, starting from the first layer until the last loss layer

$$a_l = h_l(x_l) \text{ and } x_{l+1} = a_l$$

- **Step 2.** Once done with forward propagation, follow the reverse path. Start from the last layer and for each new layer compute the gradients

$$\frac{\partial \mathcal{L}}{\partial a_l} = \left(\frac{\partial a_{l+1}}{\partial x_{l+1}}\right)^T \cdot \frac{\partial \mathcal{L}}{\partial a_{l+1}} \text{ and } \frac{\partial \mathcal{L}}{\partial \theta_l} = \frac{\partial \mathcal{L}}{\partial a_l} \cdot \left(\frac{\partial a_l}{\partial \theta_l}\right)^T$$

  - Cache computations when possible to avoid redundant operations

- **Step 3.** Use the gradients $\frac{\partial \mathcal{L}}{\partial \theta_l}$ with Stochastic Gradient Descend to train your network

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Vector with dimensions $[d_l \times 1]$

Vector with dimensions $[d_{l+1} \times 1]$

Jacobian matrix with dimensions $[d_{l+1} \times d_l]$

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Vector with dimensions $[d_{l+1} \times 1]$

Jacobian matrix with dimensions $[d_{l+1} \times d_l]$

Matrix with dimensions $[d_l \times d_{l-1}]$

Vector with dimensions $[d_l \times 1]$

Vector with dimensions $[1 \times d_{l-1}]$

Practical example and dimensionality analysis

- Layer $l-1$ has 15 neurons ($d_{l-1}=15$), l has 10 neurons ($d_l=10$) and $l+1$ has 5 neurons ($d_{l+1}=5$)
- My activation functions are $a_l = w_l x_l$ and $a_{l+1} = w_{l+1} x_{l+1}$
- The dimensionalities are *(remember $x_l = a_{l-1}$)*
  - $a_{l-1} \rightarrow [15 \times 1],\ a_l \rightarrow [10 \times 1],\ a_{l+1} \rightarrow [5 \times 1]$
  - $x_l \rightarrow [15 \times 1],\ x_{l+1} \rightarrow [10 \times 1]$
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- The gradients are
  - $\frac{\partial \mathcal{L}}{\partial a_l} \rightarrow [10 \times 5] \cdot [5 \times 1] = [10 \times 1]$
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Still, backpropagation can be slow

- Often loss surfaces are
  - non-quadratic
  - highly non-convex
  - very high-dimensional
- No real guarantee that
  - the final solution will be good
  - we converge fast to final solution
  - or that there will be convergence
- How can we protect ourselves better?

Stochastic Gradient Descend (SGD)

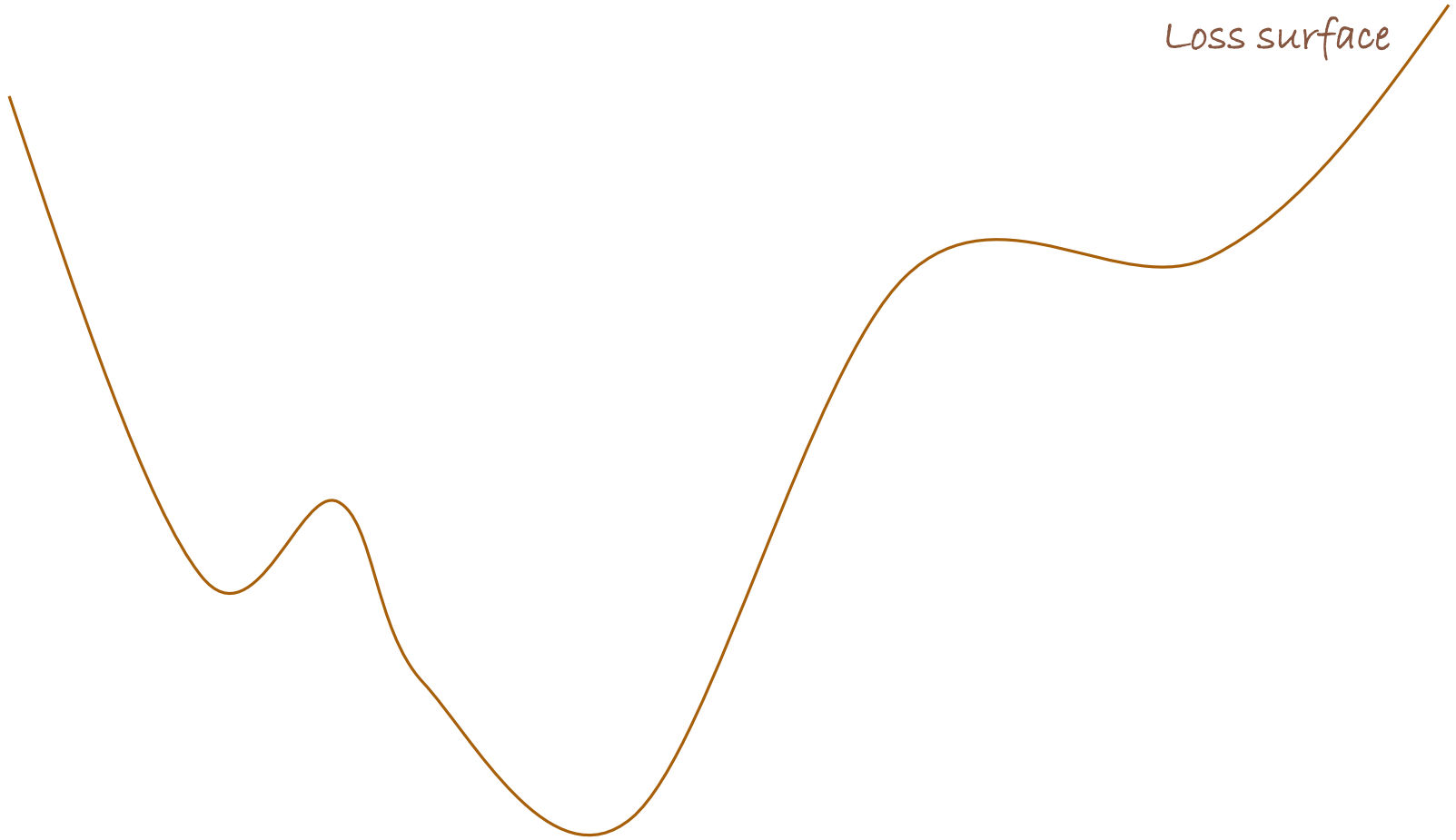
- Stochastically sample "mini-batches" from dataset D
  - The size of B_j can contain even just 1 sample

$$B_j = sample(D)$$

$$\theta^{(t+1)} = \theta^{(t)} - \frac{\eta_t}{|B_j|} \sum_{i \in B_j} \nabla_\theta \mathcal{L}_i$$

- Much faster than Gradient Descend
- Results are often better
- Can be used for dynamically changed datasets

SGD is often better



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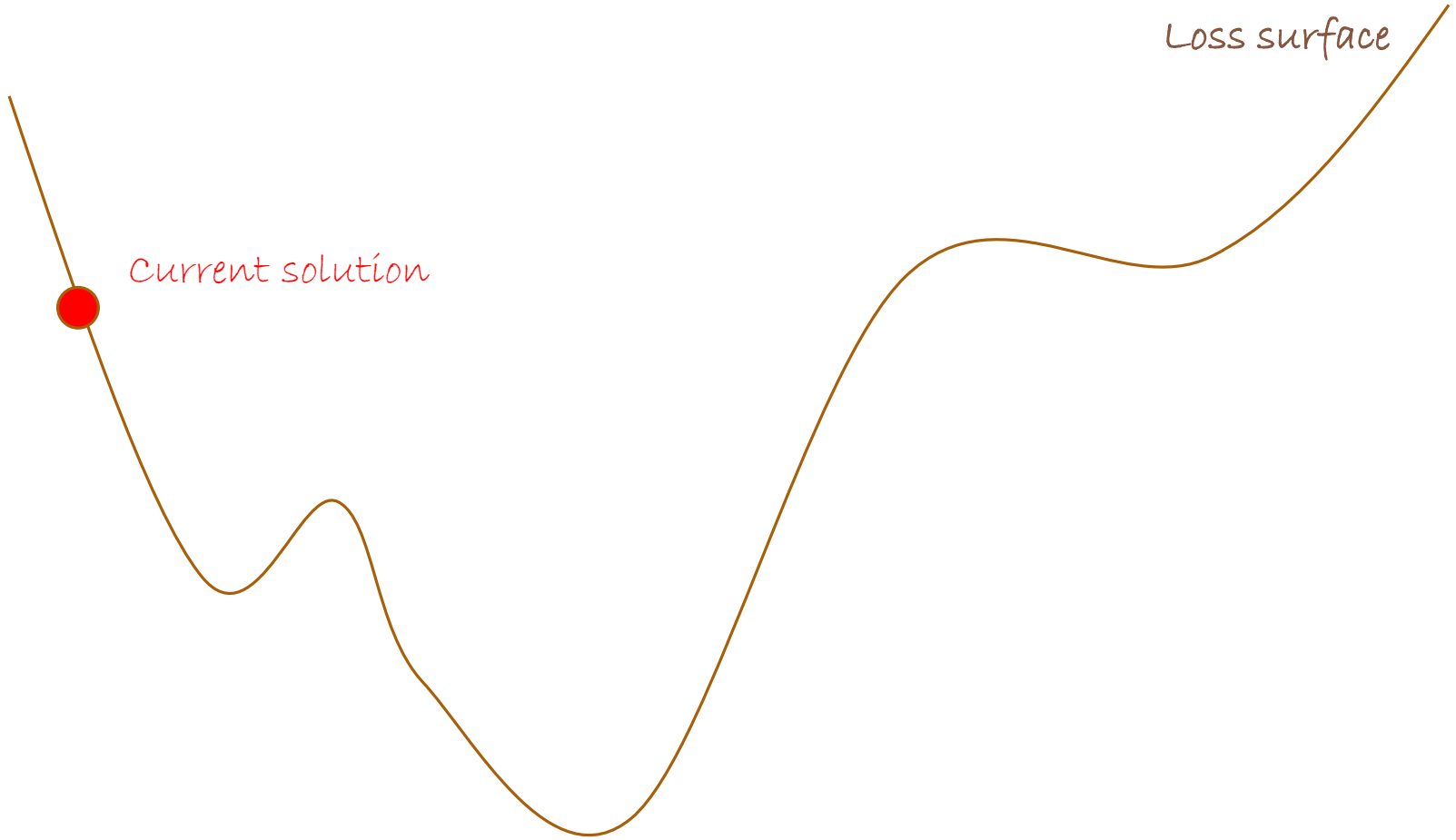

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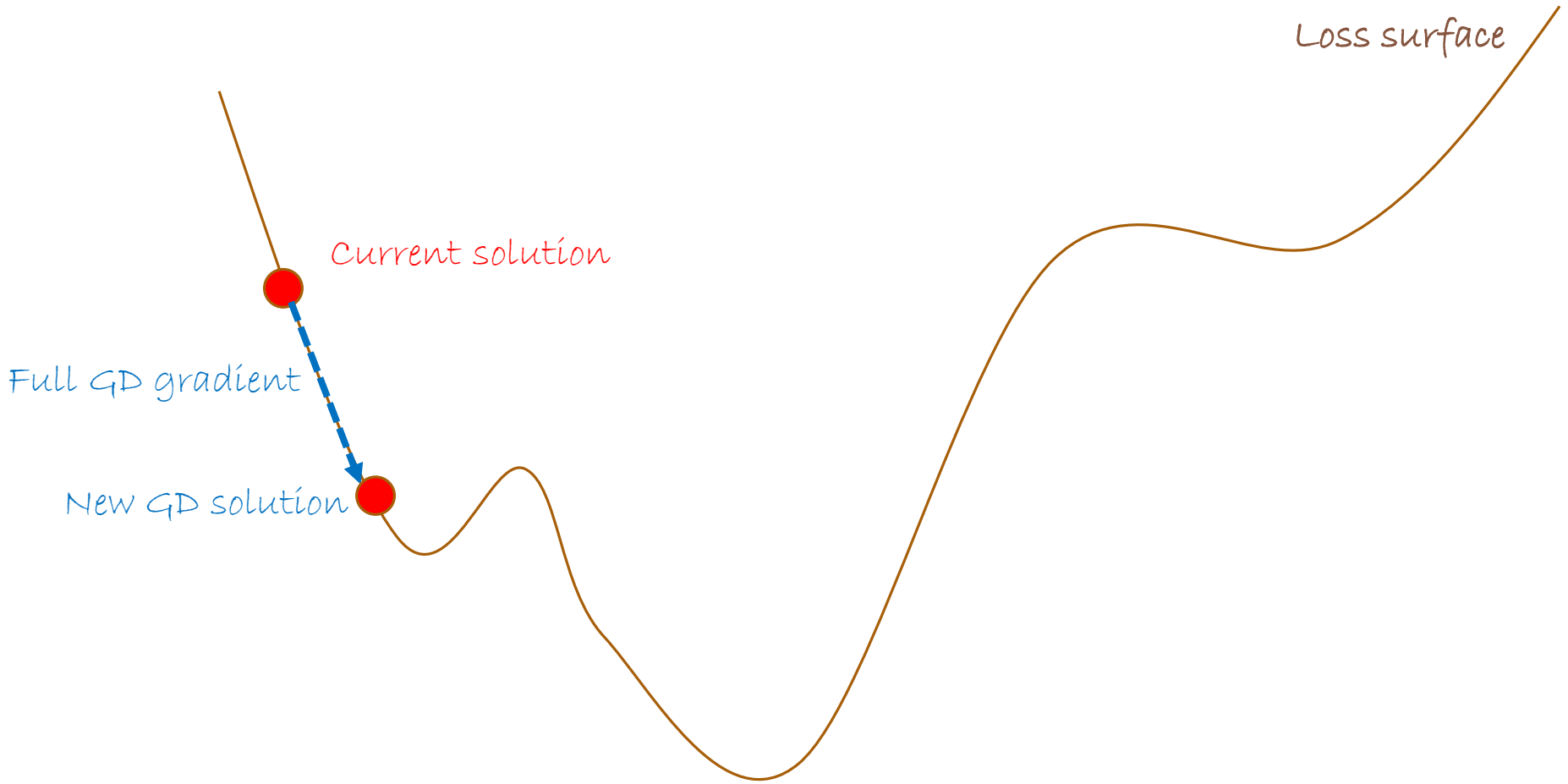

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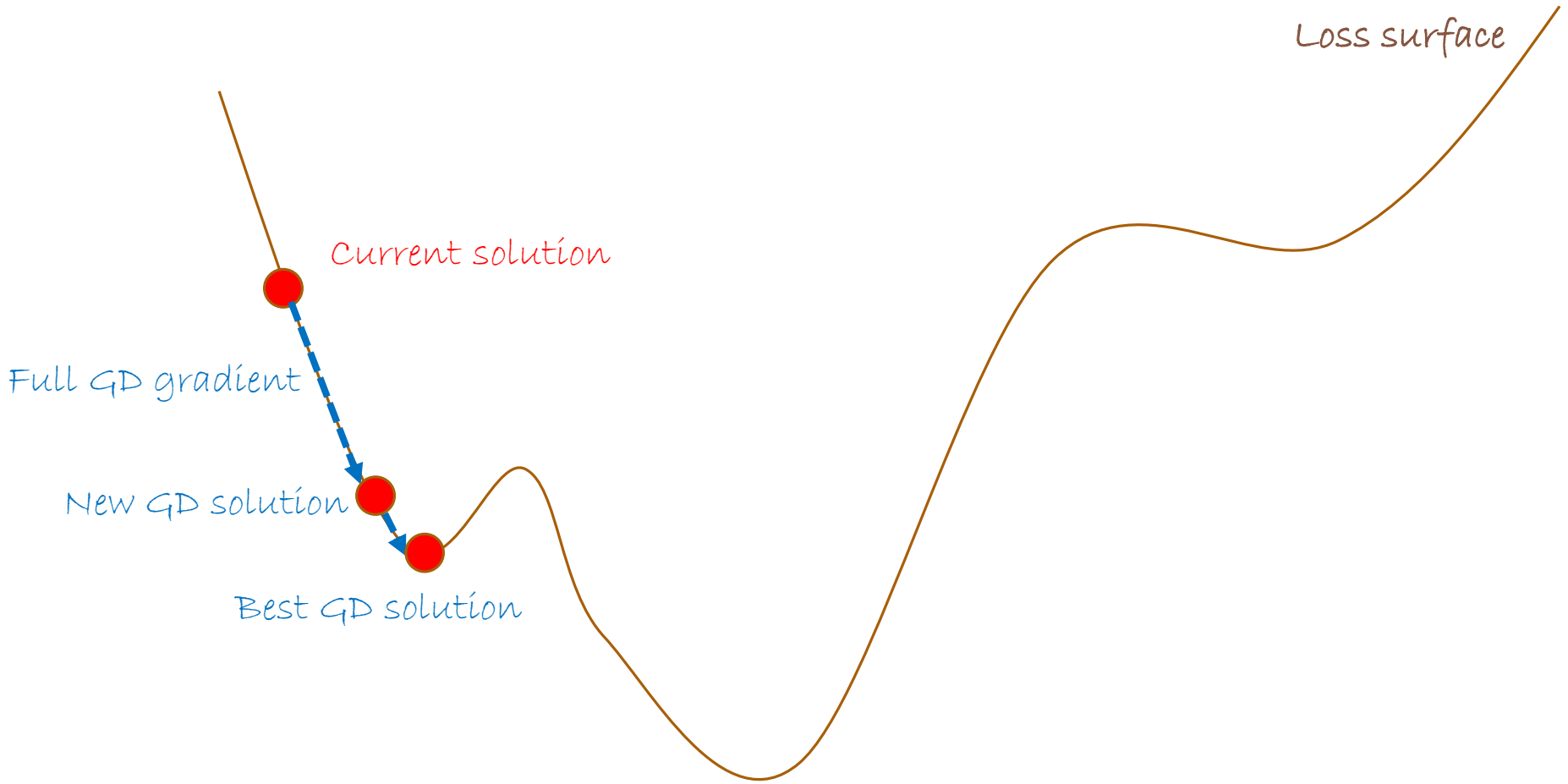

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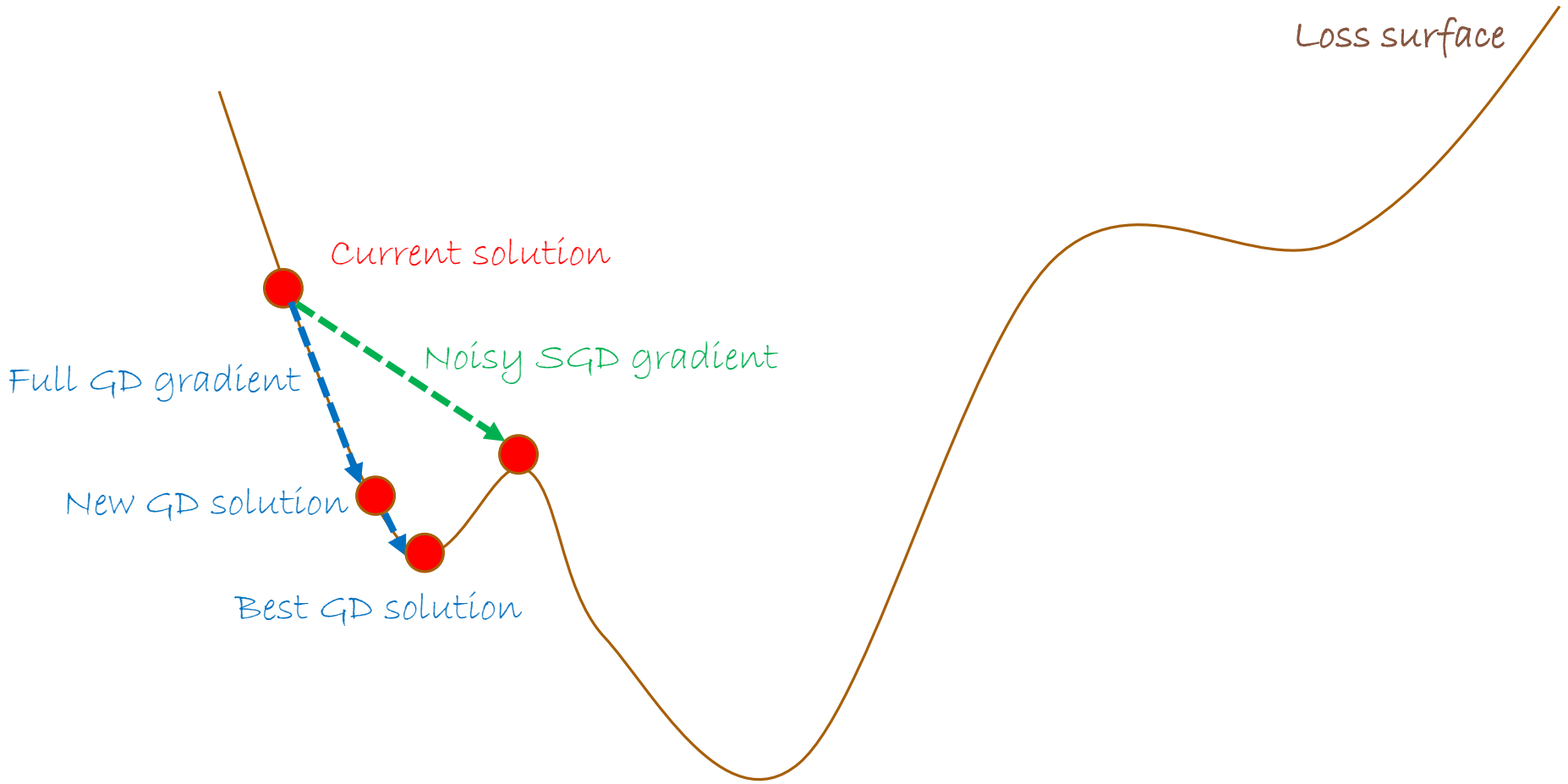

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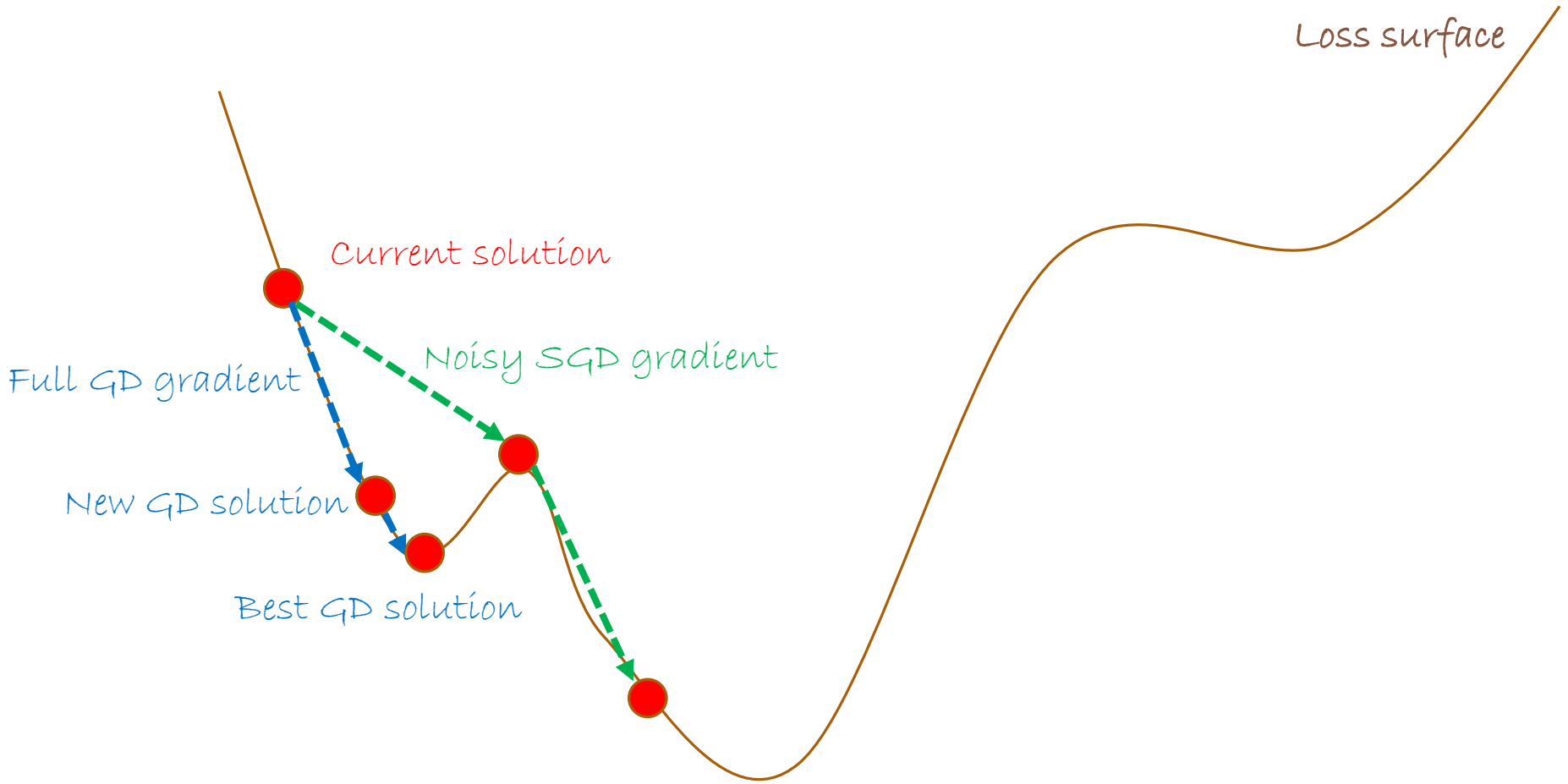

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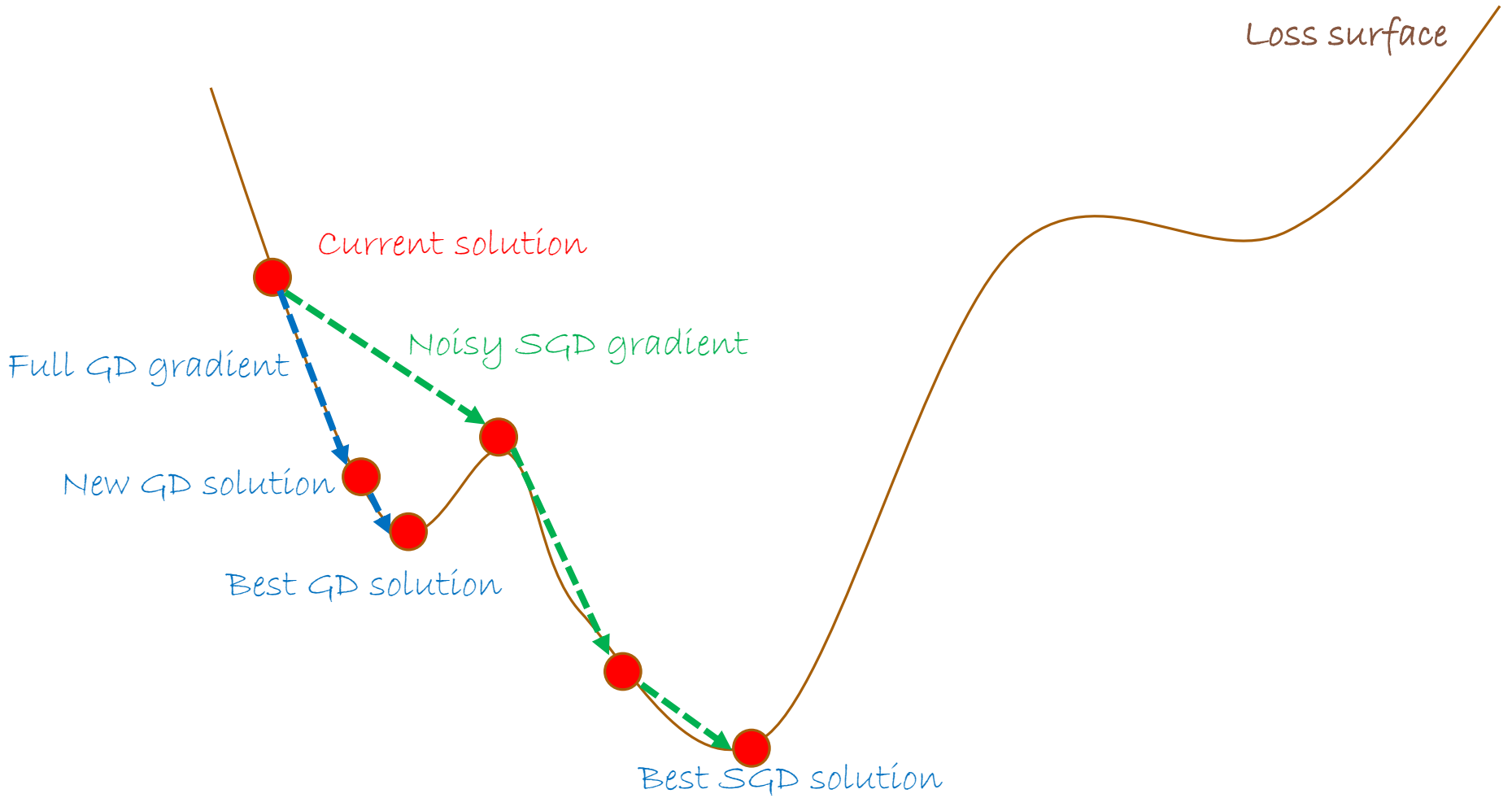

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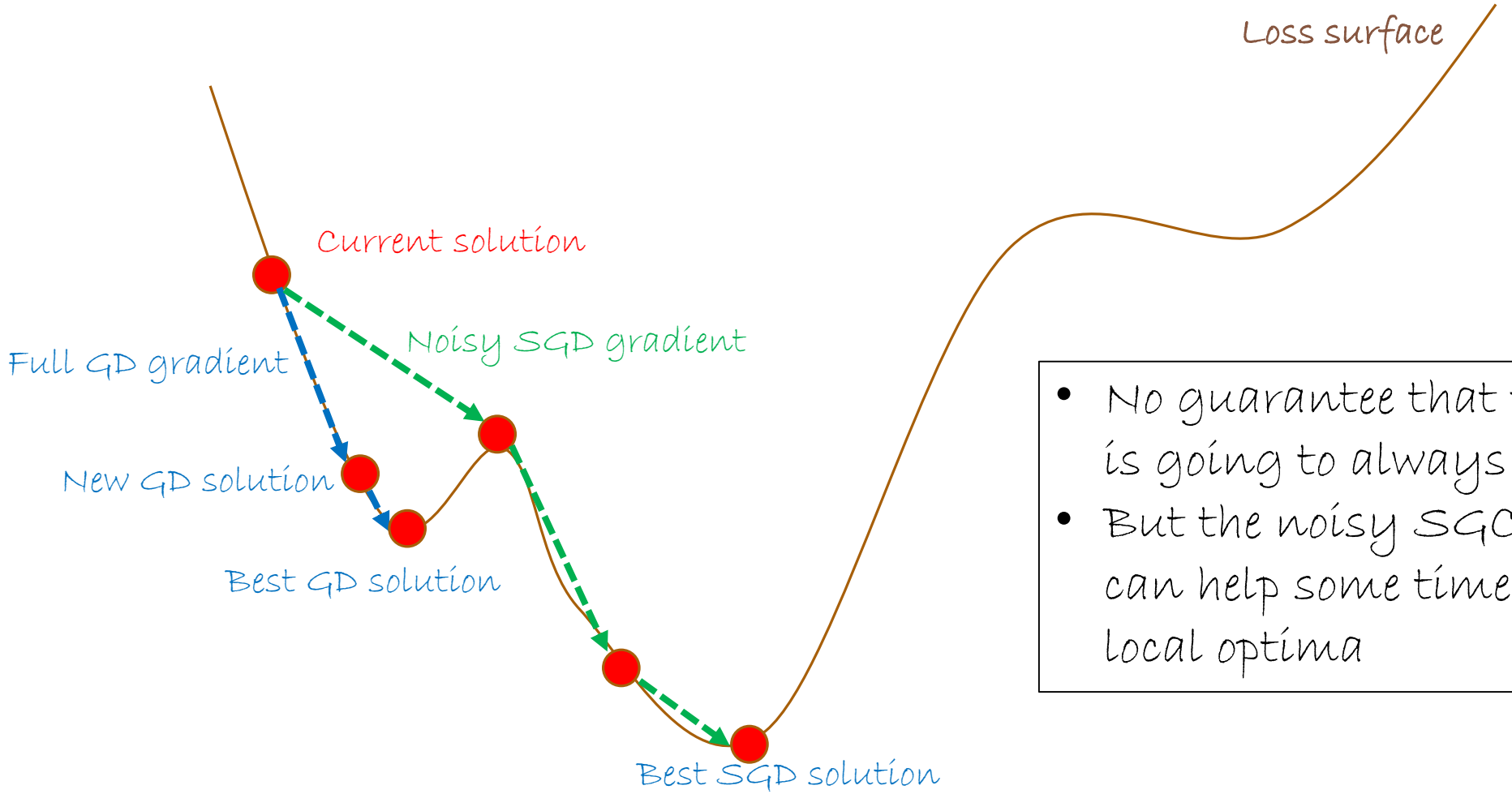
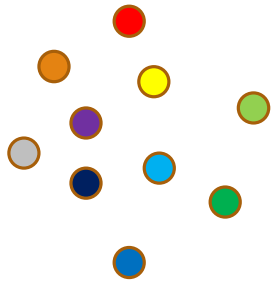


- No guarantee that this is what is going to always happen.
- But the noisy SGC gradients can help some times escaping local optima

SGD is often better

- The gradient is more “noisy”
- A noisy gradient acts as regularization
- Model does not assume that the training samples are the “absolute representative” of the input distribution
  - Traditional optimization problems: “find optimal route”
- Instead, the model assumes that the sampled training data is roughly representative
- So, model does not overfit to the particular training samples

SGD is faster



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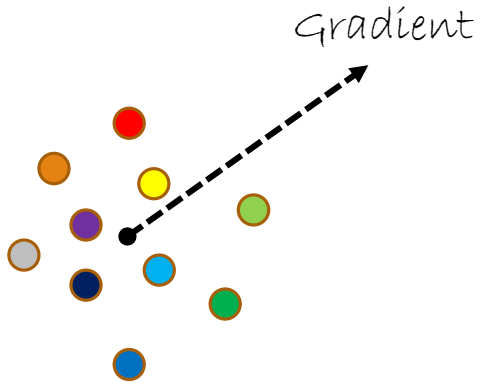

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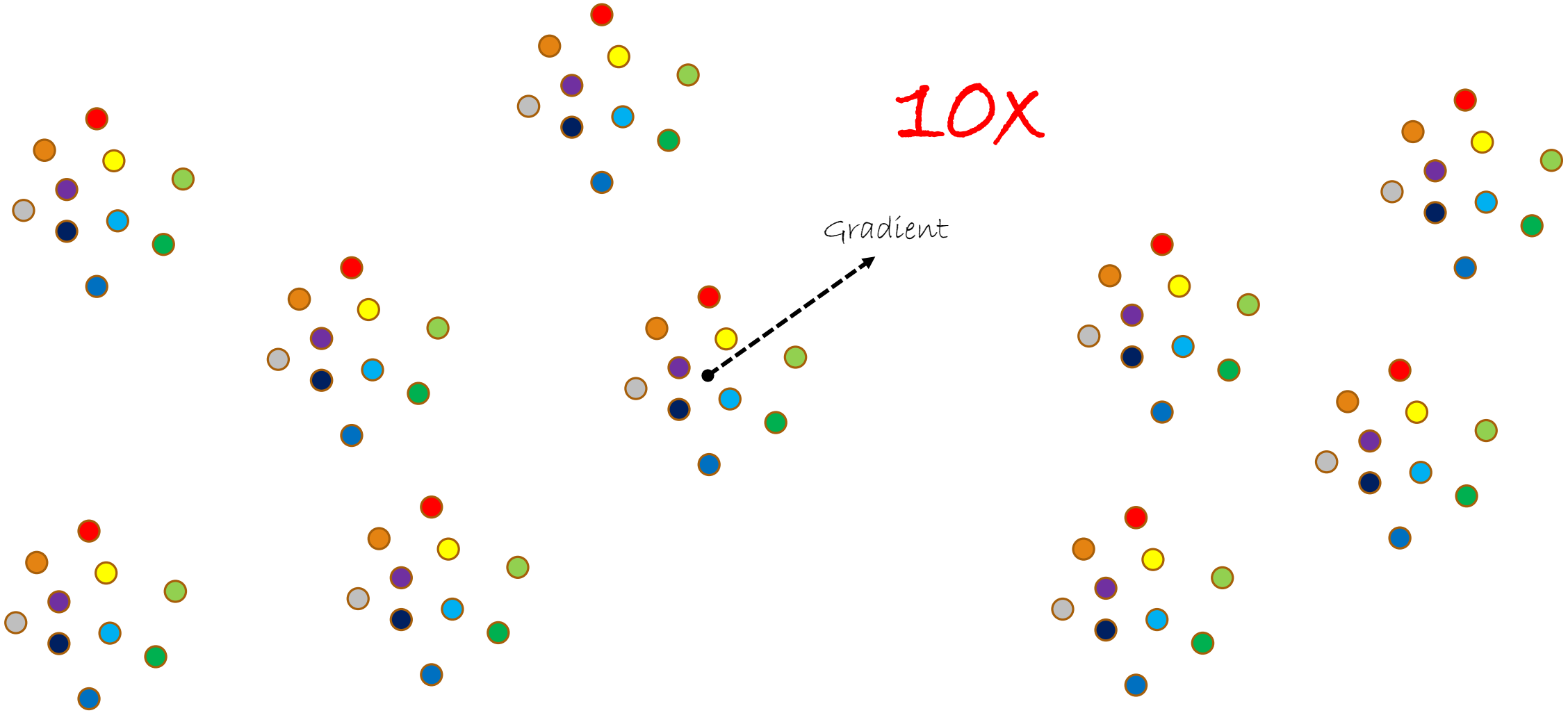

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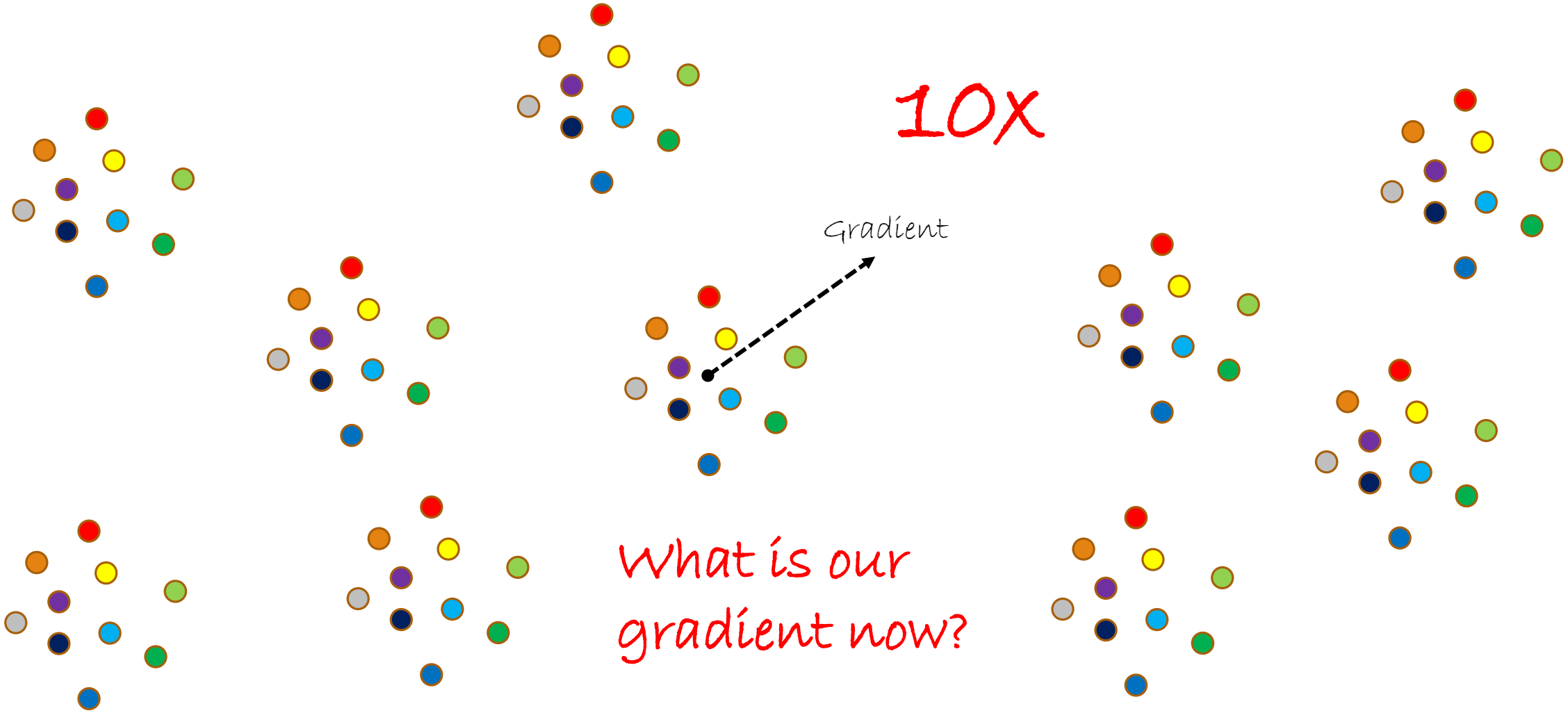

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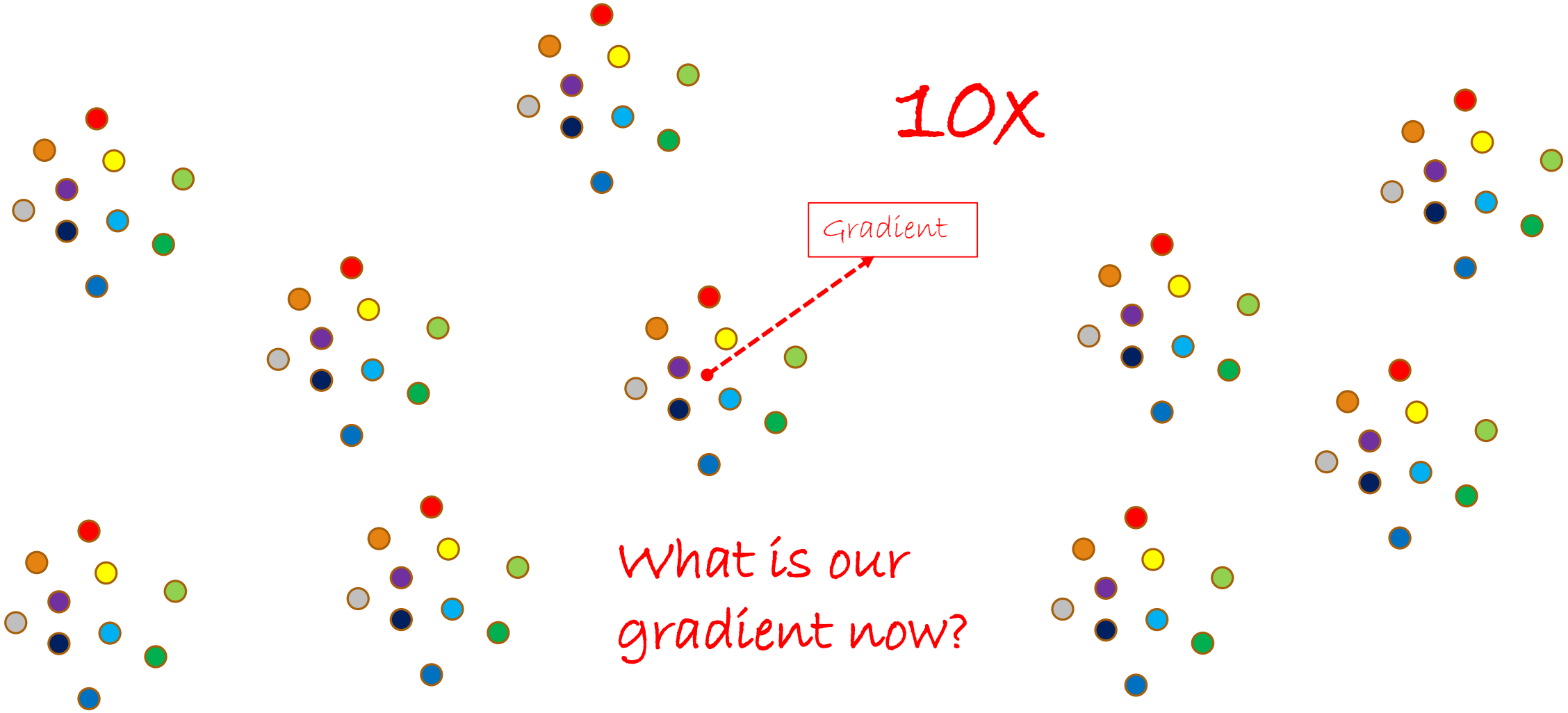


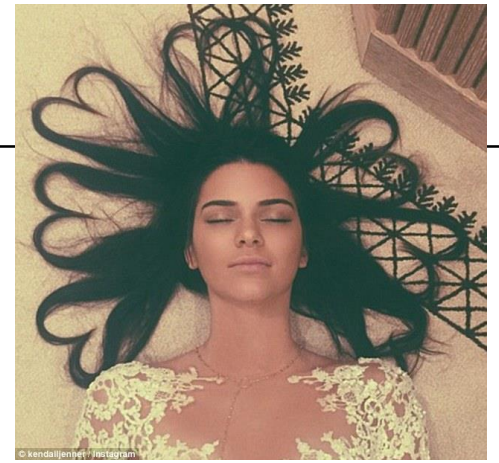
SGD is faster

- Of course in real situations data do not replicate
- However, after a sizeable amount of data there are clusters of data that are similar
- Hence, the gradient is approximately alright
- Approximate alright is great, is even better in many cases actually

SGD for dynamically changed datasets

- Often datasets are not “rigid”
- Imagine Instagram
  - Let’s assume 1 million of **new** images uploaded per week and we want to build a “cool picture” classifier
  - Should “cool pictures” from the previous year have the same as much influence?
  - No, the learning machine should track these changes
- With GD these changes go undetected, as results are averaged by the many more “past” samples
  - Past “over-dominates”
- A properly implemented SGD can track changes much better and give better models
  - [LeCun2002]

SGD for dynamically changed datasets



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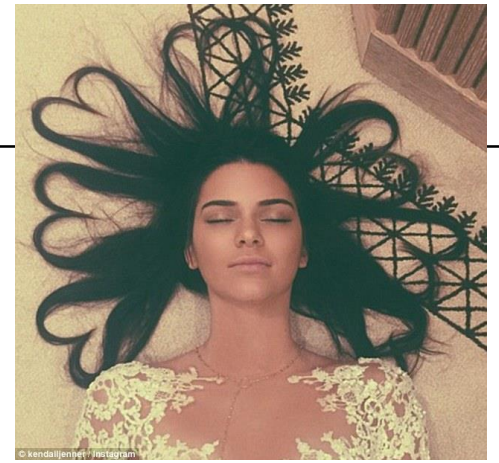

Cool this week

Cool in 2014

SGD for dynamically changed datasets

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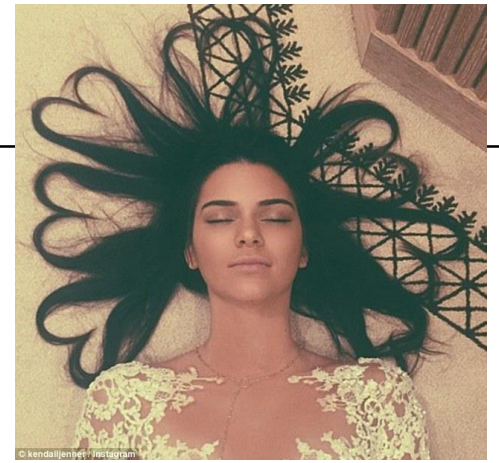


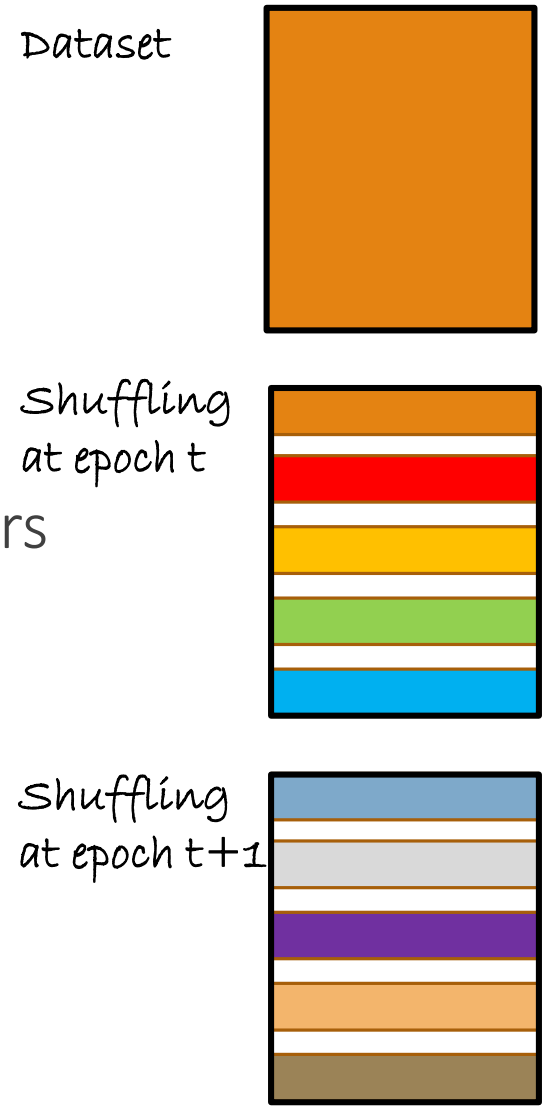
Cool this week

Cool in 2014

Cool in 2010

Shuffling examples

- Applicable only with SGD
- Choose samples with maximum information content
- Shuffle samples so that in a mini-batches the training examples are from different classes
  - As different as possible
- Prefer samples that are more likely to generate larger errors
  - Otherwise gradients will be small and learning will be slow
  - Check the errors from previous rounds and prefer “hard examples”
  - Don’t overdo it though :P, beware of outliers
- In practice, split your dataset into mini-batches
  - Each mini-batch is as class-divergent and rich as possible
  - At each new epoch create new batches with new, randomly shuffled examples



Advantages of Gradient Descend batch learning

- Conditions of convergence well understood
  - The “good noise” prevents from finding the absolutely best (for our given training dataset) solution
- Acceleration techniques can be applied
  - Second order (Hessian based) optimizations are possible
  - Measuring not only gradients, but also curvatures of the loss surface
- Simpler theoretical analysis on weight dynamics and convergence rates

In practice

- SGD is preferred to Gradient Descend
- Training is orders faster
  - In real datasets Gradient Descend is not even realistic
- Solutions are better and with better generalization
  - Important not only for efficiency, but also for dataset size scale-up
  - Much larger datasets, much better generalization
- How many samples per mini-batch?
  - Hyper-parameter, trial & error
  - Usually between 32-256 samples for image datasets

Data preprocessing & normalization

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3. Optimizing with Gradient Descend based methods

$$\theta^{(t+1)}=\theta^{(t)}-\eta_t\nabla_\theta\mathcal{L}$$

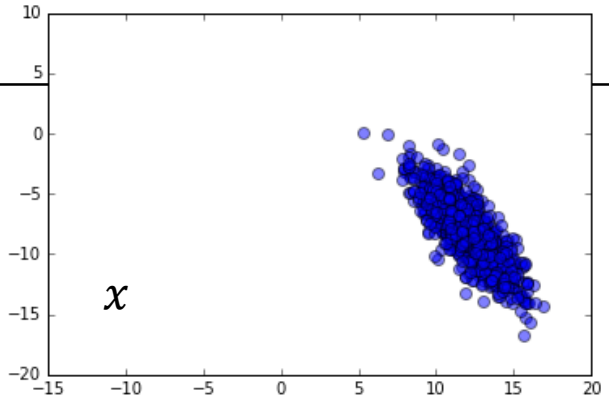
Data pre-processing

- The average of every input variable should be roughly 0
  - Convergence usually faster
  - Otherwise there is bias on the gradient direction, which slows down learning
- Scale input variables so that they have similar diagonal covariances

$$C_i = \sum_j (x_i^{(j)})^2$$

  - Similar covariances help to balance out better the rate at which the weights learn
  - Rescaling to 1 is a good choice, unless some dimensions are less important
- Input variables should be as uncorrelated as possible
  - Input variables are “more independent”, hence one can optimize them better in isolation (not jointly)
  - Caution: extreme correlation (linear dependency) might cause problems

Normalization: $N(\mu, \sigma^2) = N(0, 1)$



- Input variables follow a Gaussian distribution (roughly)
- In practice:
  - from training set compute mean and standard deviation
  - Then subtract the mean from training samples
  - Then divide the result by the standard deviation

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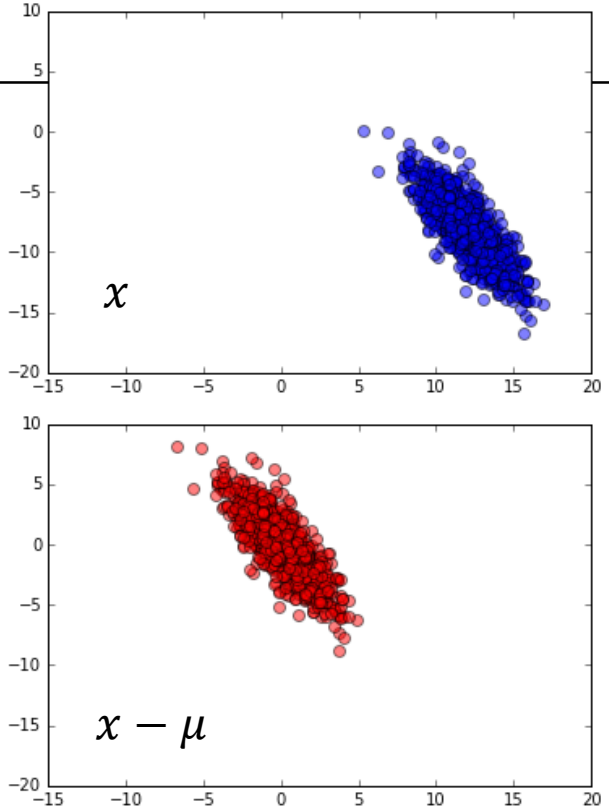

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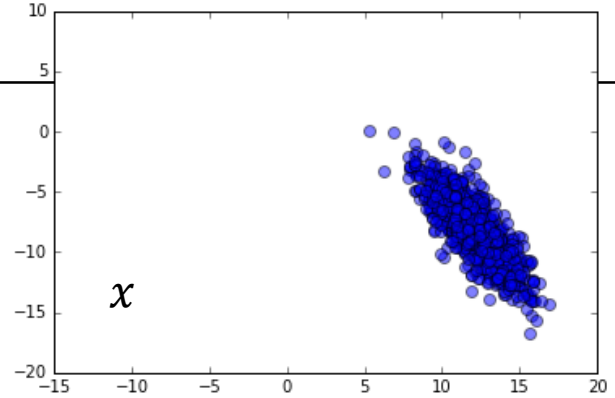
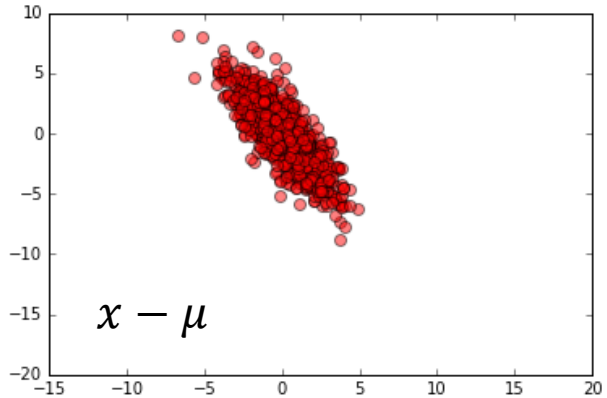
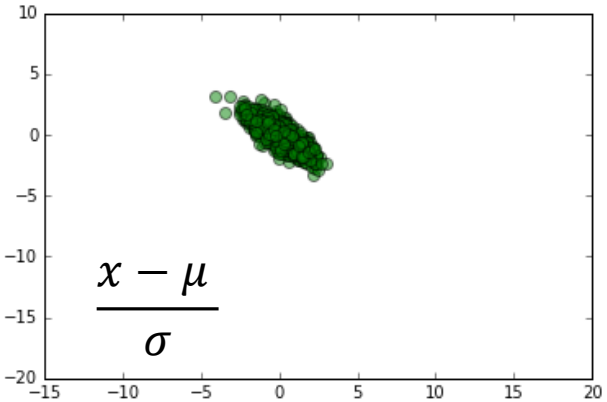






Normalization: $N(\mu, \sigma^2) = N(0, 1)$

- This normalization can be done for all input variables simultaneously
  - If they take more or less similar values, like pixels in natural images
  - Compute one (μ, σ^2) instead of as many as the input variables
- E.g. for images you can compute the general pixel average/variance
  - Or the per color channel pixel average/variance

$$(\mu_{red}, \sigma^2_{red}), (\mu_{green}, \sigma^2_{green}), (\mu_{blue}, \sigma^2_{blue})$$

- Or for every variable dimension, e.g. for every pixel R, G, B varible

PCA Whitening

- If $X = [x_1, \dots, x_N]$ and C the covariance matrix is your dataset, εigenvalues and eigenvectors are computed with SVD

$$U, \Sigma, V^T = svd(C)$$

- Then, the decorrelated (PCA-ed) version of the dataset is obtained by

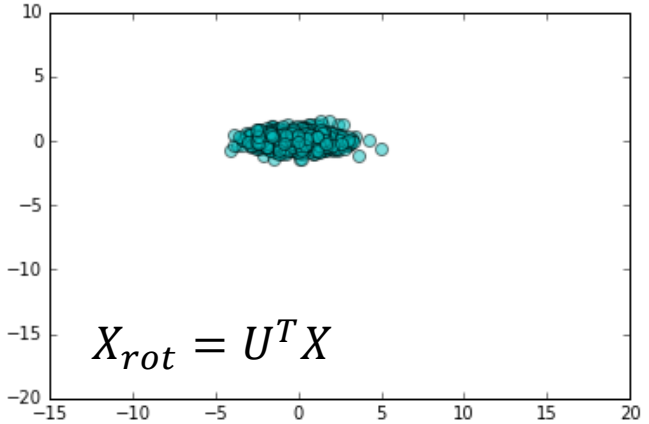
$$X_{rot} = U^T X$$

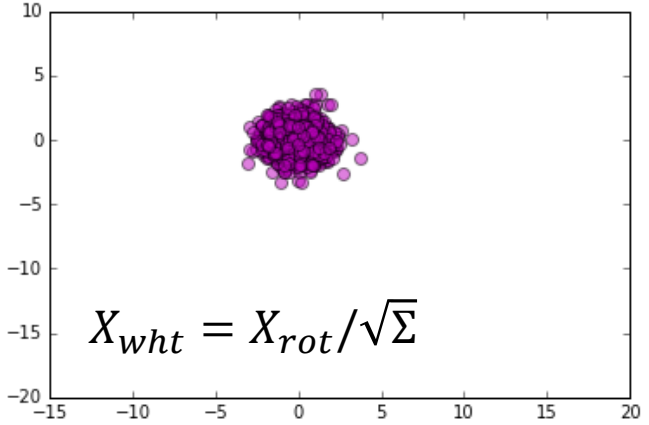
  - Few eigenvectors $U' = [u_1, \dots, u_q]$ return rotated and reduced (in dimensions) version of the data

- Scaling by the square root of eigenvalues gives the whitened data

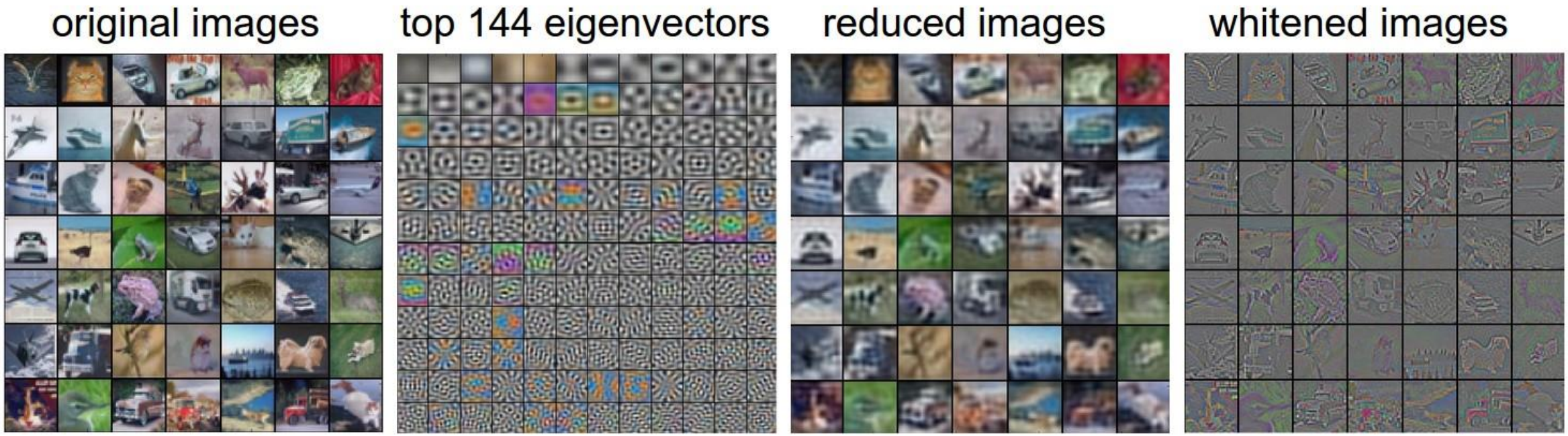
$$X_{wht} = X_{rot} / \sqrt{\Sigma}$$

- With Convolutional Neural Nets this normalization is not used that much
  - The zero mean normalization is more important





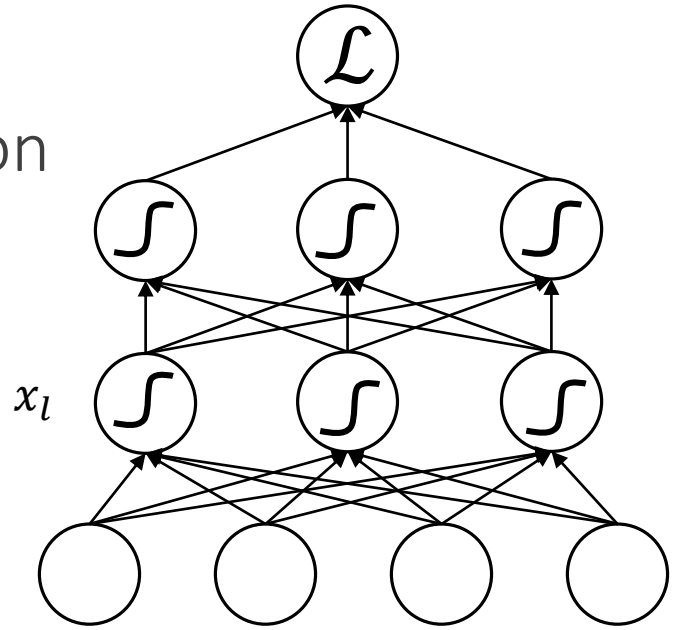
Example

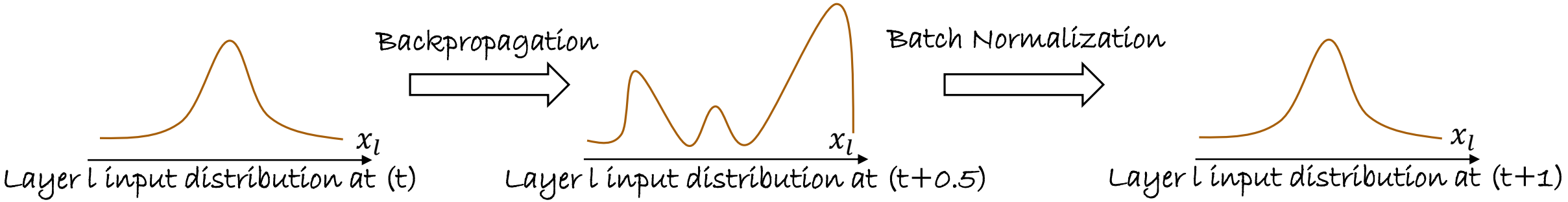


Images taken from A. Karpathy course website: http://cs231n.github.io/neural-networks-2/

Batch normalization

- Weights change → the distribution of the layer inputs changes per round
  - Covariance shift
- Normalize the layer inputs with batch normalization
  - Roughly speaking, normalize x_l to $N(0,1)$ and rescale
- Benefits
  - Neurons get activated in a near optimal "regime"
  - Gradients can be stronger, learning rates can be higher
  - Training becomes faster





Data augmentation

Original

Flip

Random crop

Contrast

Tint

Regularization

1. The Neural Network

$$a_L\left(x;\theta_{1,\ldots,\mathrm{L}}\right) = h_L\left(h_{L-1}(\ldots h_1(x,\theta_1),\theta_{L-1}),\theta_L\right)$$

2. Learning by minimizing empirical error

$$\theta^* \leftarrow \arg\min_\theta \sum_{(x,y)\subseteq(X,Y)} \ell\left(y, a_L\left(x;\theta_{1,\ldots,\mathrm{L}}\right)\right)$$

3. Optimizing with Gradient Descend based methods

$$\theta^{(t+1)} = \theta^{(t)} - \eta_t \nabla_\theta \mathcal{L}$$

Regularization

- Neural networks typically have thousands, if not millions of parameters
  - Usually, the dataset size smaller than the number of parameters
- Overfitting is a grave danger
- Proper weight regularization is crucial to avoid overfitting

$$\theta^* \leftarrow \arg\min_\theta \sum_{(x,y)\subseteq(X,Y)} \ell(y, a_L(x; \theta_{1,\ldots,L})) + \lambda\Omega(\theta)$$

- Possible regularization methods
  - ℓ_2-regularization
  - ℓ_1-regularization
  - Dropout

ℓ_2-regularization

- ℓ_2-regularization is one of the most important techniques

$$\theta^* \leftarrow \arg\min_\theta \sum_{(x,y)\subseteq(X,Y)} \mathcal{L}(y, a_L(x; \theta_{1,\ldots,L})) + \frac{\lambda}{2}\sum_l \|\theta_l\|^2$$

- The ℓ_2-regularization can pass inside the gradient descend update rule

$$\theta^{(t+1)} = \theta^{(t)} - \eta_t(\nabla_\theta \mathcal{L} + \lambda\theta_l) \Longrightarrow$$
$$\theta^{(t+1)} = (1 - \lambda\eta_t)\theta^{(t)} - \eta_t \nabla_\theta \mathcal{L}$$

- λ is usually about $10^{-1}, 10^{-2}$
- Good practice: divide by the number of samples in your (mini-) batch

$$(1 - \lambda\eta_t)\theta^{(t)}$$

if your loss is also averaged by the number of samples

ℓ_2-regularization

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"Weight decay", because weights get smaller

- λ is usually about $10^{-1}, 10^{-2}$
- Good practice: divide by the number of samples in your (mini-) batch

$$(1-\lambda\eta_t)\theta^{(t)}$$

if your loss is also averaged by the number of samples

ℓ_1-regularization

- ℓ_1-regularization is one of the most important techniques

$$\theta^* \leftarrow \arg\min_\theta \sum_{(x,y)\subseteq(X,Y)} \mathcal{L}(y, a_L(x; \theta_{1,\ldots,L})) + \frac{\lambda}{2}\sum_l \|\theta_l\|$$

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$$\theta^{(t+1)} = \theta^{(t)} - \lambda\eta_t \frac{\theta^{(t)}}{|\theta^{(t)}|} - \eta_t \nabla_\theta \mathcal{L}$$

- ℓ_1-regularization induces model sparsity
  - Weights are more likely to become 0 with larger λ

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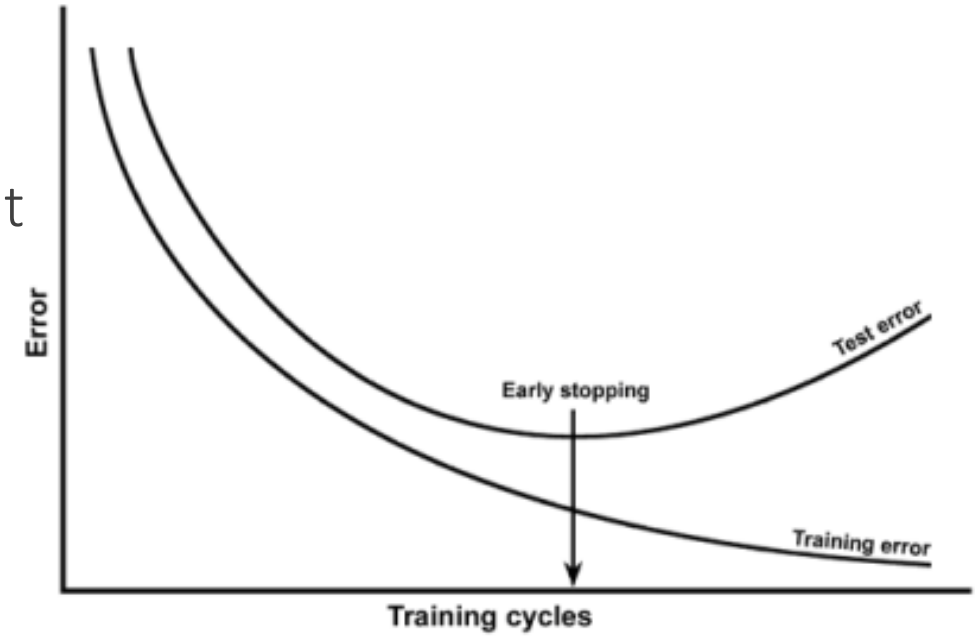
Sign function

- ℓ_1-regularization induces model sparsity
  - Weights are more likely to become 0 with larger λ

Early stopping

- To tackle overfitting another popular technique is early stopping
- Monitor performance on a separate validation set
- Training the network will decrease training error, as well validation error (although with a slower rate usually)
- Stop when validation error starts increasing
  - This quite likely means the network starts to overfit



Dropout

- During training setting activations randomly to 0
  - Neurons sampled at random from a Bernoulli distribution with $p = 0.5$
- Effectively, a different architecture at every training epoch
  - Reduced network, as some nodes do not contribute to final score
- Benefits
  - Reduces complex co-adaptations or co-dependencies between neurons
  - No “free-rider” neurons that rely on others
  - Every neuron becomes more robust
  - Overall, decreases significantly overfitting
  - Also, improves significantly training speed
- At test time all neurons are used
  - Neuron activations reweighted by p
- Particularly popular in computer vision, speech recognition

Architectural details

1. The Neural Network

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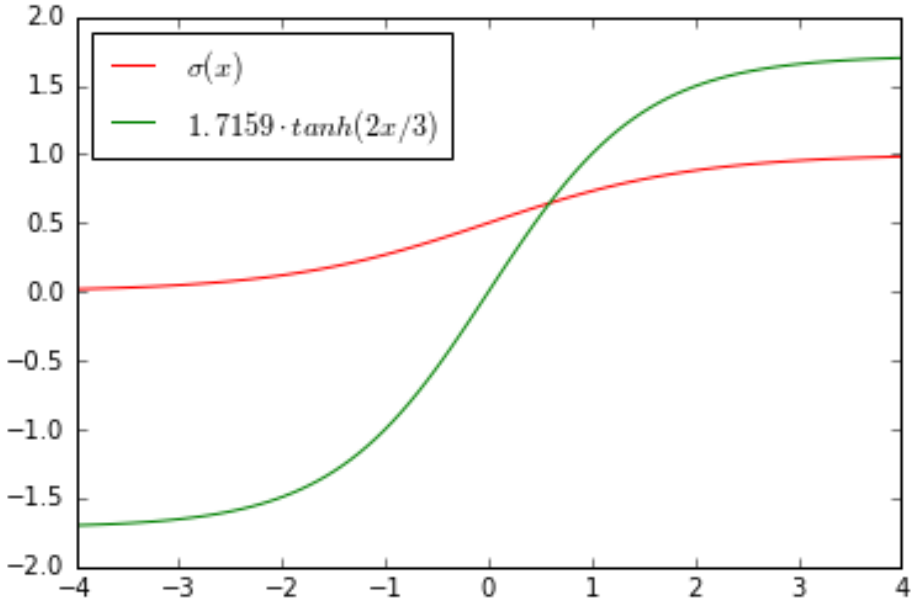
Sigmoid-like activation functions

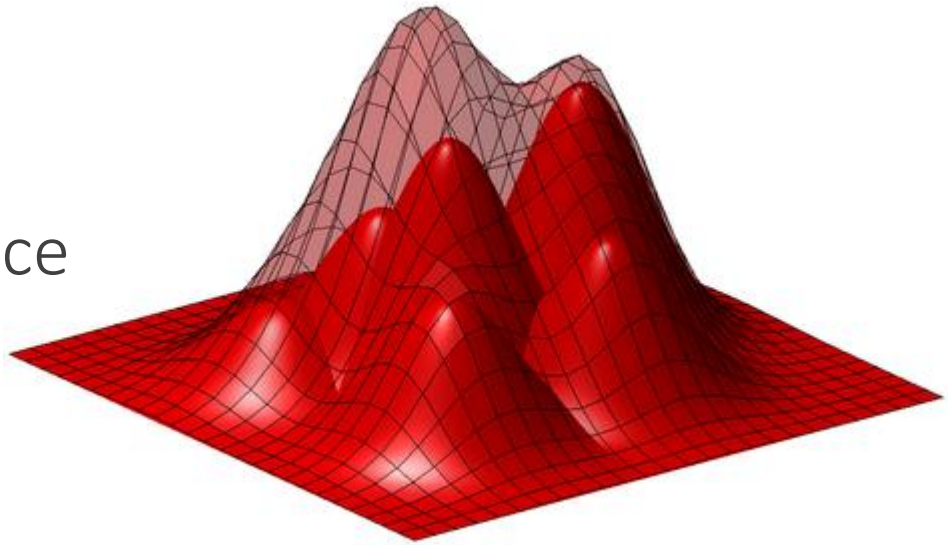
- Straightforward sigmoids are not a very good idea
- Symmetric sigmoids, like tanh, converge faster
- A recommended sigmoid is $a = h(x) = 1.7159 \tanh(\frac{2}{3}x)$
  - A $\tanh$ can be computationally expensive, maybe approximate by ratio of polynomials
- You can add a linear term to avoid flat areas

$$a = h(x) = \tanh(x) + \beta x$$



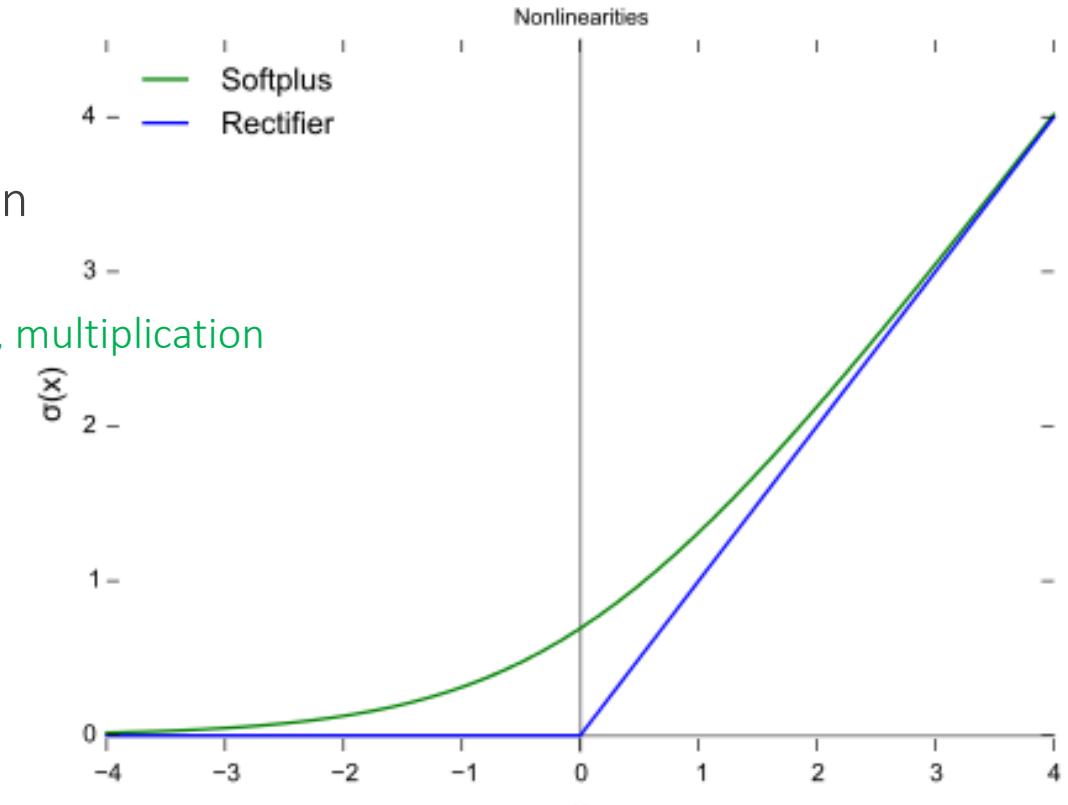
RBFs vs "Sigmoids"

- RBF: $a = h(x) = \sum_j u_j \exp\left(-\beta_j \left(x - w_j\right)^2\right)$
- Sigmoid: $a = h(x) = \sigma(x) = \frac{1}{1+e^{-x}}$
- Sigmoids can cover the full feature space
- RBF's are much more local in the feature space
  - Can be faster to train but with a more limited range
  - Can give better set of basis functions
  - Preferred in lower dimensional spaces

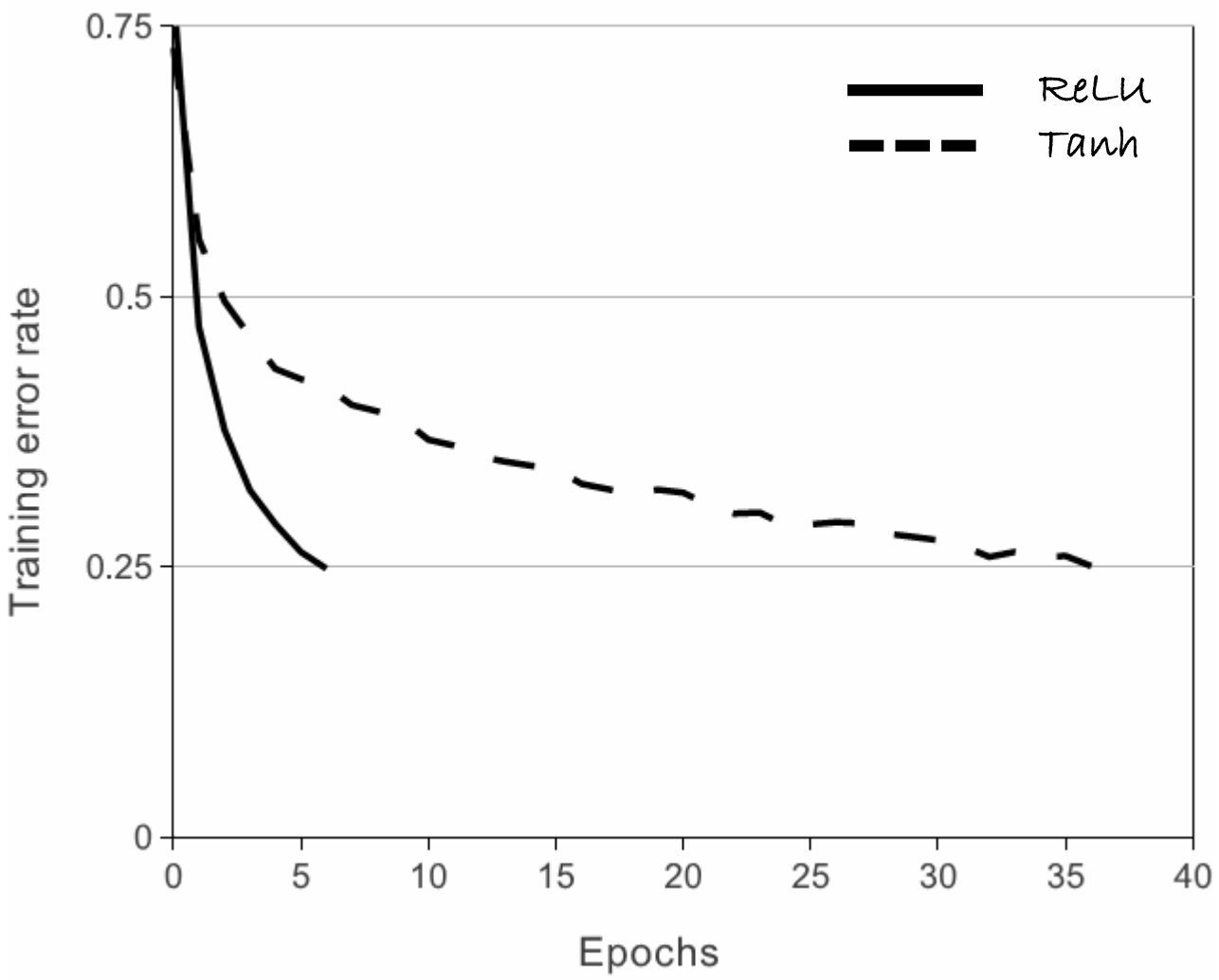


Rectified Linear Unit (ReLU) module (Alexnet)

- Activation function $a = h(x) = \max(0, x)$
- Gradient wrt the input $\frac{\partial a}{\partial x} = \begin{cases} 0, if\ x \leq 0 \\ 1, if x > 0 \end{cases}$
- Very popular in computer vision and speech recognition
- Much faster computations, gradients
  - No vanishing or exploding problems, only comparison, addition, multiplication
- People claim biological plausibility
- Sparse activations
- No saturation
- Non-symmetric
- Non-differentiable at 0
- A large gradient during training can cause a neuron to "die". Higher learning rates mitigate the problem



ReLU convergence rate



Other ReLUs

- Soft approximation (softplus): $a = h(x) = \ln(1 + e^x)$
  - Gradient is the sigmoid $\frac{\partial a}{\partial x} = \sigma(\chi)$
- Noisy ReLU: $a = h(x) = \max(0, \mathrm{x} + \varepsilon), \varepsilon \sim N(0, \sigma(\mathrm{x}))$
- Leaky ReLU: $a = h(x) = \begin{cases} x, if\ x > 0 \\ 0.01x\ otherwise \end{cases}$
- Parametric ReLu: $a = h(x) = \begin{cases} x, if\ x > 0 \\ \beta x\ otherwise \end{cases}$
  - parameter β is trainable

Architectural hyper-parameters

- Number of hidden layers
- Number of neuron in each hidden layer
- Type of activation functions
- Type and amount of regularization

Number of hidden units, number of hidden layers

- Getting these hyper-parameters is dataset dependent
- Start small and gradually increase complexity
- With no regularization the plot of number of hidden units vs. generalization performance graph will be U-shaped
- E.g. start with a few hidden layers, 2 or 3
- And a few dozen hidden units per layer and see if performance is reasonable
  - Start increasing the number of layers and see if performance improves
  - Start increasing the number of hidden units and see if performance improves

Use ℓ_2-regularization!

- In general though ℓ_2-regularization is more important!!
- It's alright if you have a deep or wide network
- If there is the ℓ_2-regularization is strong enough, your network will generally not overfit

Learning rate

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Learning rate

- The right learning rate is important for fast convergence
  - Too strong, the gradients overshoot and bounce
  - Too weak, the gradients are too small to influence the parameters → slow training
- Sometimes learning rate per weight is advantageous
  - Some weights are near convergence, others not
- If weights are shared, a good idea is the learning rate to be proportional to the square root of the number of connections sharing the weight
- Adaptive learning rates are also possible, based on the errors observed
  - [Sompolinsky1995]

Learning rate schedules

- Constant
  - Learning rate remains the same for all epochs
- Step decay
  - Decrease (e.g. $\eta_t/2$ or $\eta_t/10$) every T number of epochs
- Inverse decay $\eta_t = \frac{\eta_0}{1+\varepsilon t}$
- Exponential decay $\eta_t = \eta_0 e^{-\varepsilon t}$
- Generally step decay is simple, intuitive, it works well and does not require tuning extra hyper-parameters, other than when to decrease η_t

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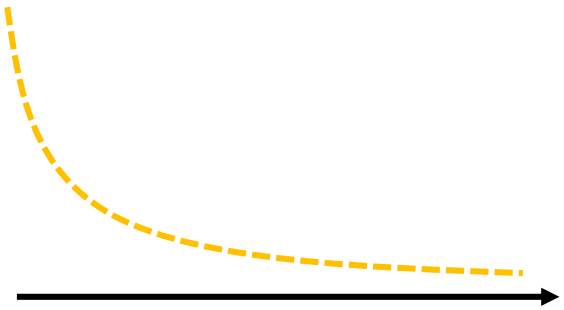

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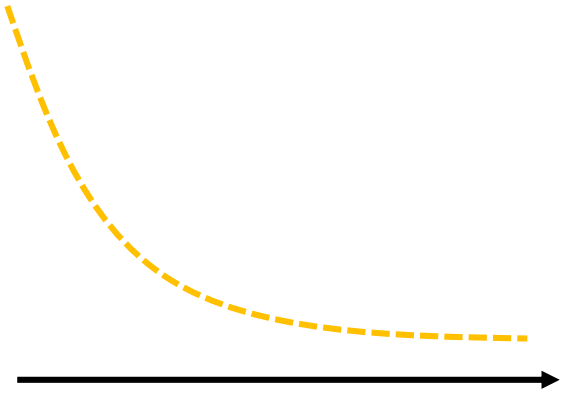

Learning rate in practice

- Try several log-spaced values $10^{-1}, 10^{-2}, 10^{-3}, \ldots$ on a smaller set
  - Then, you can narrow it down from there around where you get the lowest error
- You can decrease the learning rate every 10 (or some other value) full training set epochs
  - Although this highly depends on your data

Weight initialization

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3. Optimizing with Gradient Descend based methods

$$\theta^{(t+1)}=\theta^{(t)}-\eta_t\nabla_\theta\mathcal{L}$$

Weight initialization

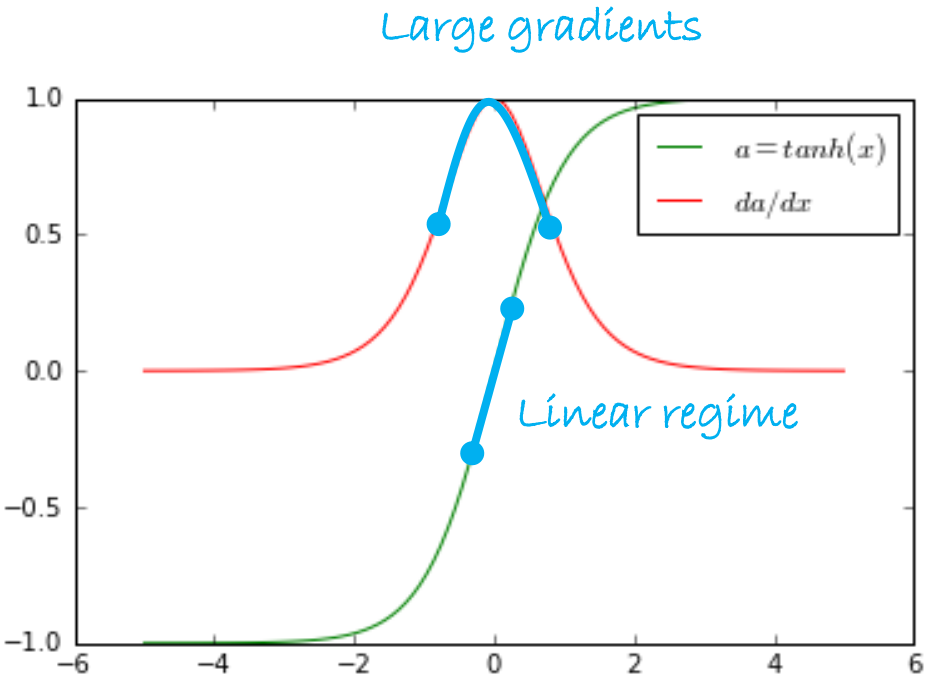
- There are few contradictory requirements
- Weights need to be small enough
  - e.g. around the origin ($\vec{\mathbf{0}}$) for symmetric functions (tanh, sigmoid)
  - the activation functions operate near their linear regime → large gradients → faster training
- Weights need to be large enough
  - The generated gradients are also large enough → faster training

Weight initialization

- Weights must be initialized to preserve the variance of the activations during the forward and backward computations, especially for deep learning
  - All neurons operate in their full capacity
- Good practice: initialize weights to be asymmetric, e.g. no same values for different weights (like all $\vec{\mathbf{0}}$)
  - Otherwise all neurons generate the same gradient, no real change
  - Alternatively, initialize to $\vec{\mathbf{0}}$ but break some node to node connections to create asymmetries
- Generally, Initialization must be coordinated with the choice of non-linear activation functions and data normalization

Weight initialization for sigmoid-like neurons

- For tanh initialize weights from $\left[-\sqrt{\frac{6}{d_{l-1}+d_l}}, \sqrt{\frac{6}{d_{l-1}+d_l}}\right]$
  - d_{l-1} is the number of input variables to the tanh layer and d_l is the number of the output variables
- For a sigmoid $\left[-4 \cdot \sqrt{\frac{6}{d_{l-1}+d_l}}, 4 \cdot \sqrt{\frac{6}{d_{l-1}+d_l}}\right]$



Weight initialization for ReLUs

- For ReLU's you also want to initialize the weights so the neurons have similar variances
- Currently the suggested practice is to fill in the weights with random samples draw from

$$\mathrm{w} \sim N\left(0, \sqrt{2/d}\right)$$

where d is the number of neurons in the input [HeICCV2015]

Loss functions

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Multi-class classification

- Our samples contains only one class
  - There is only one correct answer per sample
- Negative log-likelihood (cross entropy) + Softmax

$\mathcal{L}(\theta; x, y) = -\sum_{c=1}^{C} y_c \log a_L^c$ for all classes $c = 1, \dots, C$

- Hierarchical softmax when C is very large
- Hinge loss (aka SVM loss)

$$\mathcal{L}(\theta; x, y) = \sum_{\substack{c=1 \\ c \neq y}}^{C} \max(0, a_L^c - a_L^y + 1)$$

- Squared hinge loss

Is it a cat? Is it a horse? …




Multi-class, multi-label classification

- Each sample can have many correct answers
- Hinge loss and the likes
  - Also sigmoids would also work
- Each output neuron is independent
  - "Does this contain a car, yes or no?"
  - "Does this contain a person, yes or no?"
  - "Does this contain a motorbike, yes or no?"
  - "Does this contain a horse, yes or no?"

- Instead of "Is this a car, motorbike or person?"
  - $p(car|x) = 0.55, p(m/bike|x) = 0.25, p(person|x) = 0.15, p(horse|x) = 0.05$
  - $p(car|x) + p(m/bike|x) + p(person|x) + p(horse|x) = 1.0$

Regression

- The good old sum of squared errors

$$\mathcal{L}(\theta; x, y) = \frac{1}{2}|y - a_L|_2^2$$

- Or the ℓ_1 distance

$$\mathcal{L}(\theta; x, y) = \sum_j |y_j - a_L^j|$$

Even better optimizations

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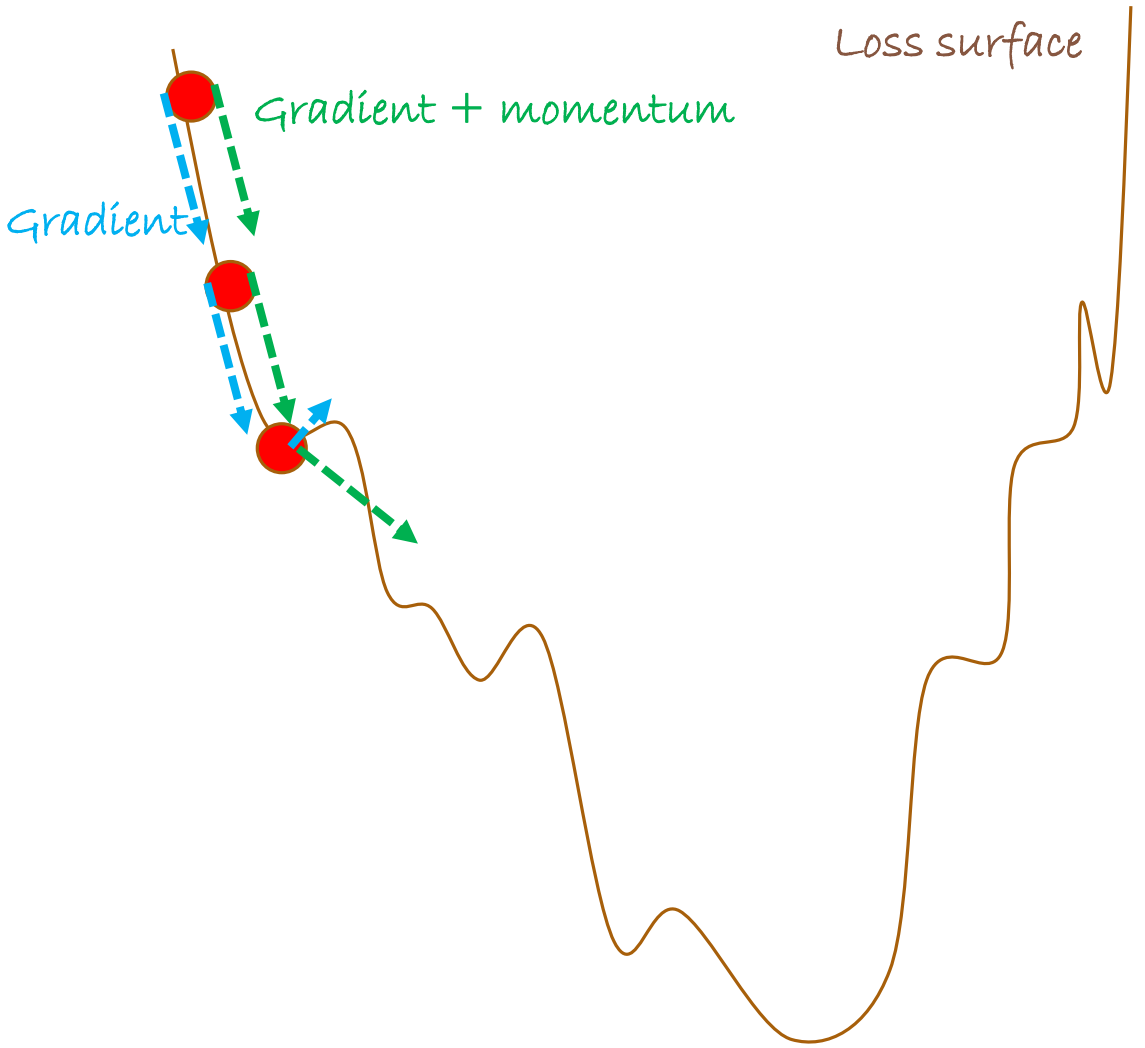
Momentum

- Instead of switching gradients all the time, maintain some "momentum" from the previous parameters

$$u_\theta = \gamma\theta^{(t)} - \eta_t \nabla_\theta \mathcal{L}$$
$$\theta^{(t+1)} = \theta^{(t)} + u_\theta$$

- Gradients and learning are more robust, faster convergence
- Nice "physics"-based interpretation
  - Instead of updating the position of the "ball", we update the velocity, which will update the position

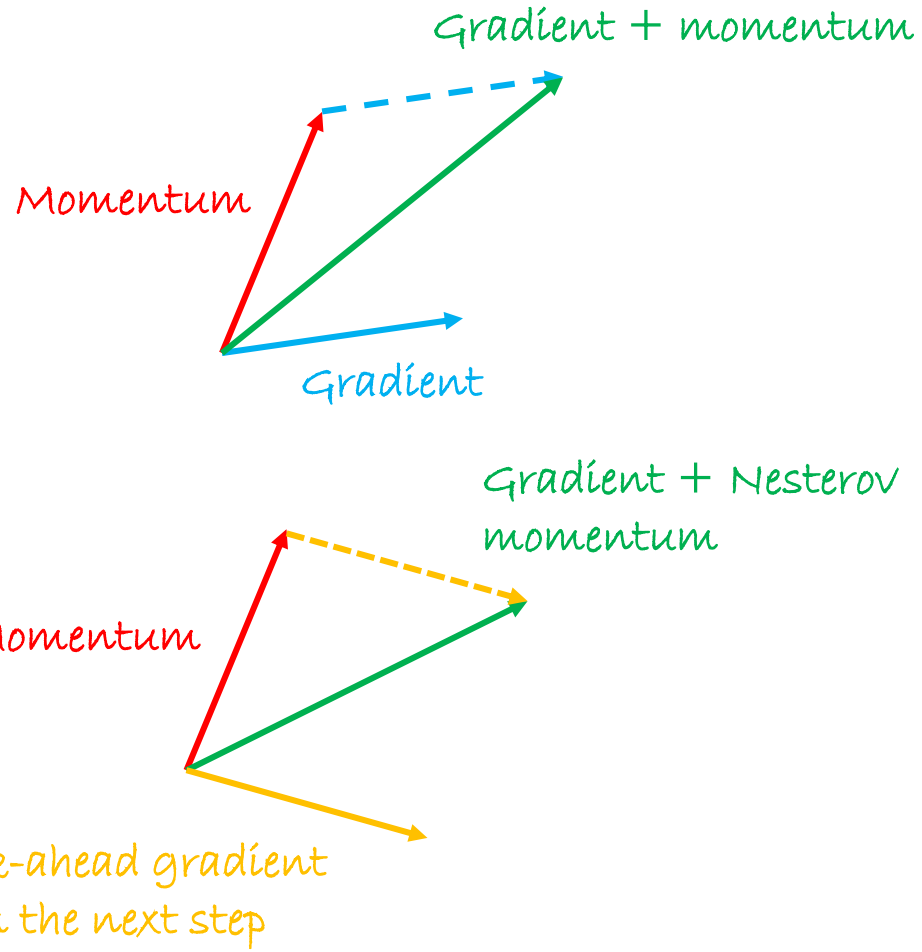


Nesterov Momentum

- Use the future gradient instead of the current gradient

$$u_\theta = \gamma\theta^{(t)} - \eta_t \nabla_\theta \mathcal{L}$$
$$\theta^{(t+1)} = \theta^{(t)} + u_\theta$$

- Better theoretical convergence
- Generally works better with Convolutional Neural Networks



Second order optimizations

- Normally we update all weights with same “aggressiveness”
  - Yet, some parameters could enjoy more “teaching”
  - While others are already about there
- Second-order methods adapt the learning according to the per parameter behavior

$$\theta^{(t+1)} = \theta^{(t)} - H_{\mathcal{L}}^{-1}\eta_t \nabla_\theta \mathcal{L}$$

- $H_{\mathcal{L}}$ is the Hessian matrix of $\mathcal{L}$ containing all second-order derivatives

$$H_{\mathcal{L}}^{ij} = \frac{\partial \mathcal{L}}{\partial \theta_i \partial \theta_j}$$

Second order optimization methods in practice

- Computing the inverse of the Hessian with thousands of parametesr is usually very expensive
- Instead approximations are sough for, e.g. the L-BFGS algorithm
  - Keeps memory of gradients to approximate the inverse Hessian
- However, L-BFGS works alright with Batch Gradient Descend
  - What about SGD?
- In practice SGD with a good momentum works alright

Per parameter adaptive optimization

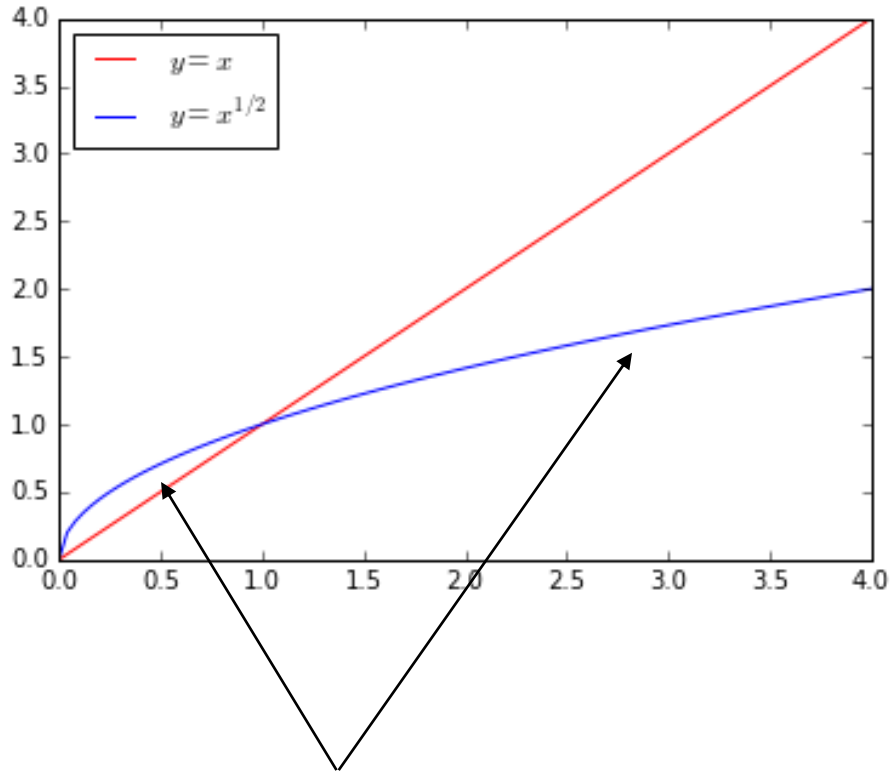
- Adagrad [Duchi2011]
- RMSprop
- Adam [Kingma2014]

Adagrad [Duchi2011]

- Schedule
  - $m_j = \sum_\tau (\nabla_\theta \mathcal{L}_j)^2 \implies \theta^{(t+1)} = \theta^{(t)} - \eta_t \frac{\nabla_\theta \mathcal{L}}{\sqrt{m}+\varepsilon}$
  - ε is a small number to avoid division with 0
  - Gradients become gradually smaller and smaller

RMSprop

- Schedule
  - $m_j = \alpha \sum_{\tau=1}^{t-1} (\nabla_\theta \mathcal{L}_j)^2 + (1-\alpha) \nabla_\theta^{(t)} \mathcal{L}_j \quad \Longrightarrow \quad \theta^{(t+1)} = \theta^{(t)} - \eta_t \frac{\nabla_\theta \mathcal{L}}{\sqrt{m}+\varepsilon}$
- α is a decay hyper-parameter
- Similar like Adagrad, but uses a moving average of the squared gradients
- When gradients are too large (maybe too "noisy" loss surface)
  - Updates are tamed
- When gradients are too small (maybe stuck in flat loss surface ravine)
  - Updates become more aggressive

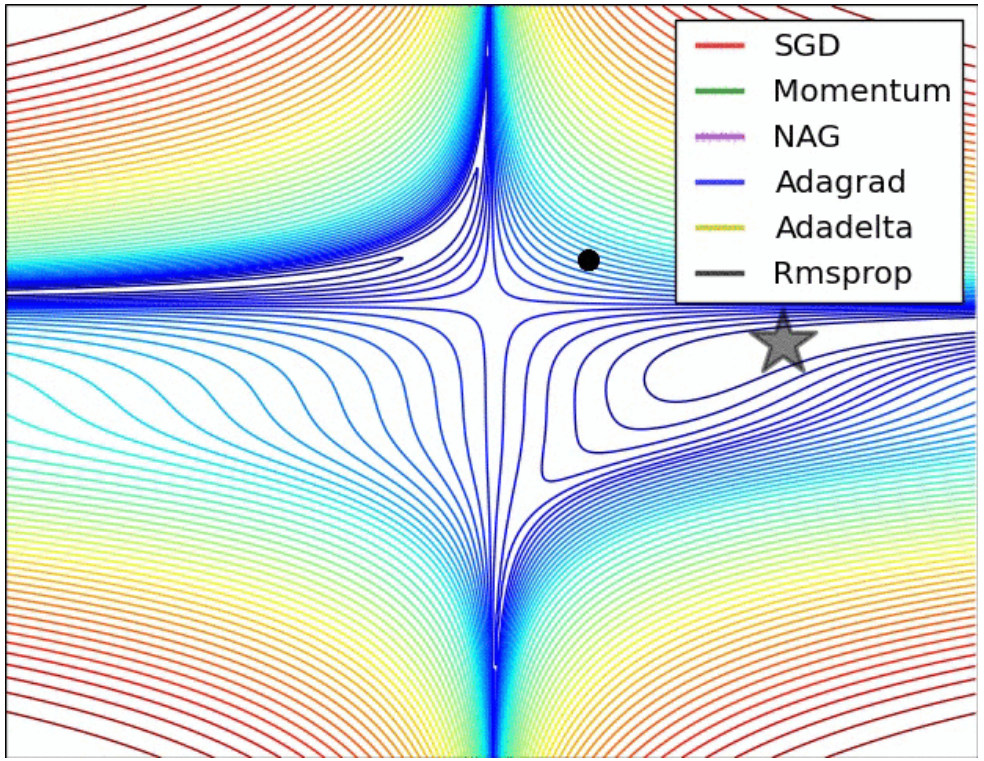


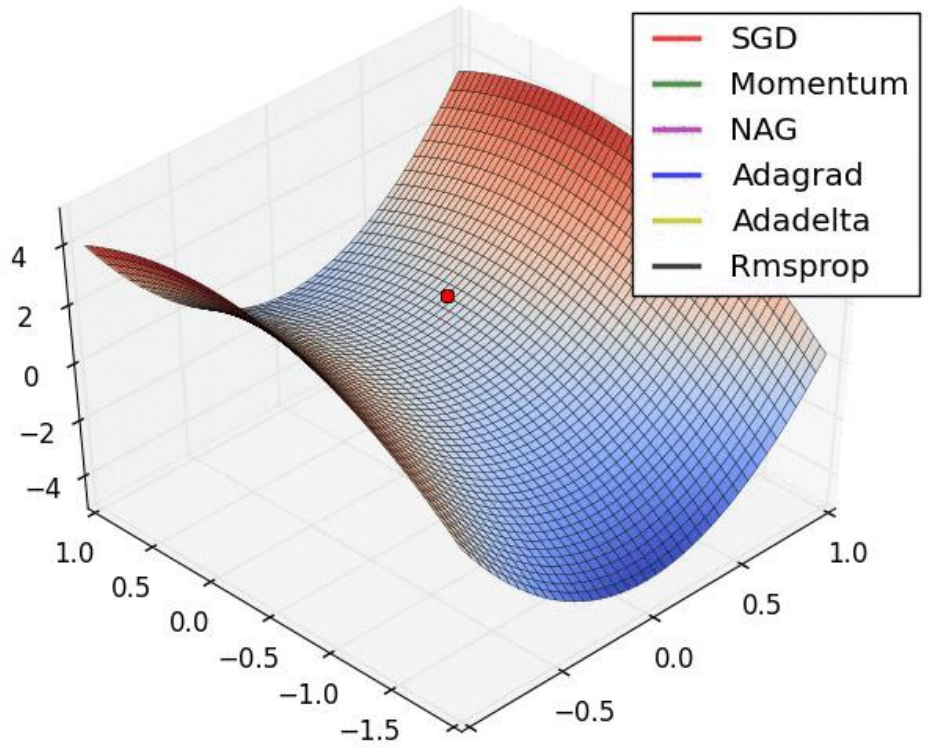
Square rooting boosts small values while suppresses large values

Adam [Kingma2014]

- $m_j = \sum_\tau (\nabla_\theta \mathcal{L}_j)^2$
- $\theta^{(t+0.5)} = \beta_1 \theta^{(t)} + (1-\beta_1)\nabla_\theta \mathcal{L}$
- $v^{(t+0.5)} = \beta_2 v^{(t)} + (1-\beta_2) m$
- $\theta^{(t+1)} = \theta^{(t)} - \eta_t \frac{\theta^{(t+0.5)}}{\sqrt{v^{(t+0.5)}} + \varepsilon}$
- Similar to RMSprop with momentum
- Recommended values: $\beta_1 = 0.9, \beta_2 = 0.999, \varepsilon = 10^{-8}$

Visual overview





Picture credit: Alec Radford

Good practice

- Preprocess the data to have 0 mean
  - Either normalize to have standard deviation 1 or the inputs to lie in the range [-1, 1]
- Initialize weights according to you activations functions
  - For ReLU initialize from $N(0, \sqrt{\frac{2}{d}})$, d is the number of input neurons
- Always use ℓ_2-regularization and dropout
- Use batch normalization

Babysitting Deep Nets

1. The Neural Network

$$a_L\left(x;\theta_{1,\ldots,\mathrm{L}}\right)=h_L\left(h_{L-1}(\ldots h_1(x,\theta_1),\theta_{L-1}),\theta_L\right)$$

2. Learning by minimizing empirical error

$$\theta^*\leftarrow\arg\min_\theta\sum_{(x,y)\subseteq(X,Y)}\mathcal{L}(y,a_L\left(x;\theta_{1,\ldots,\mathrm{L}}\right))$$

3. Optimizing with Gradient Descend based methods

$$\theta^{(t+1)}=\theta^{(t)}-\eta_t\nabla_\theta\mathcal{L}$$

Babysitting Deep Nets

- Check your gradients
- Check that in the first round you get a random loss
- Check network with few samples
  - Turn off regularization. You should predictably overfit and have a 0 loss
  - Turn or regularization. The loss should increase
- Have a separate validation set
  - Compare the curve between training and validation sets
  - There should be a gap, but not too large

Summary

- How to defining our model and optimize it in practice
- Data preprocessing and normalization
- Optimization methods
- Regularizations
- Architectures and architectural hyper-parameters
- Learning rate
- Weight initializations
- Good practices

Next lecture

- What are the Convolutional Neural Networks?
- Why are they so important for Computer Vision?
- How do they differ from standard Neural Networks?
- How can we train a Convolutional Neural Network?