Deep Learning & Applied AI

Stochastic gradient descent

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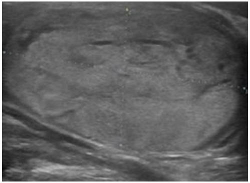
Recap

In deep learning, we deal with highly parametrized models called deep neural networks:

$$f_{\boldsymbol{\Theta}}(\mathbf{x}) = \mathbf{y}$$

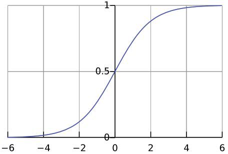
Recap: Logistic regression

What if we want to predict a category instead of a value?

$f_\Theta($  $) = \{0, 1\}$

General idea: Modify the loss to minimize over categorical values.

$$\ell_\Theta(\{x_i, y_i\}) = -\sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b))$$



Recap: Logistic regression

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(a x_i + b)) = (1 - \sigma(a x_i + b)) x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system that we can solve easily.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	nonlinear optimization

Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

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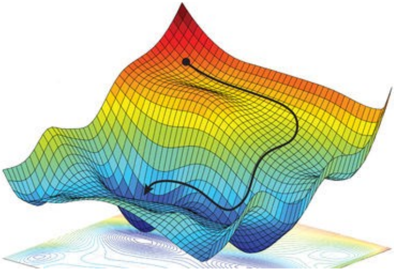

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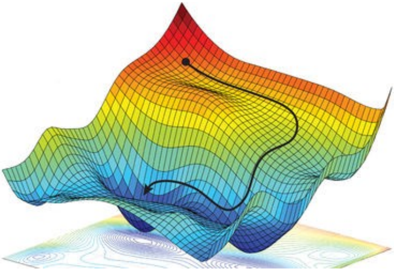

Overall idea: Move where the function decreases the most.

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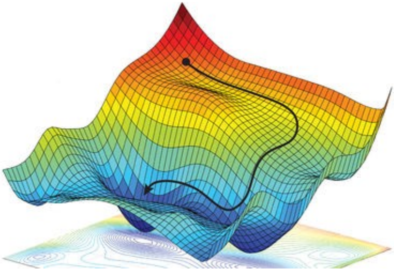

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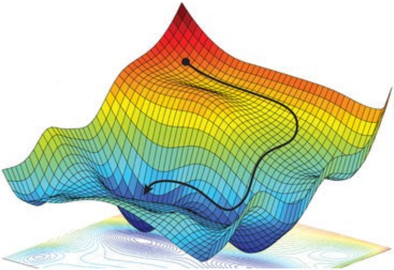

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3. Stop when a minimum is reached.

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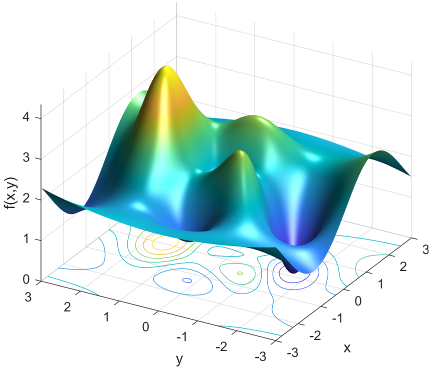

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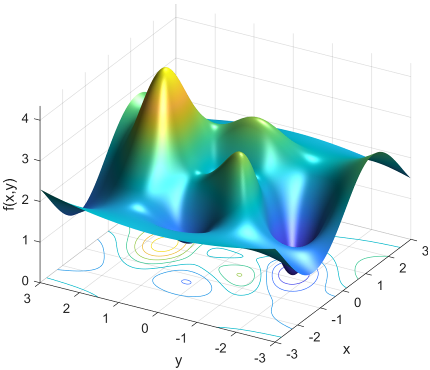

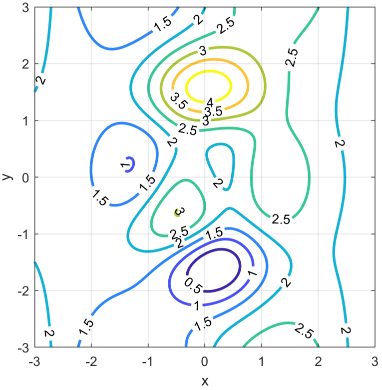

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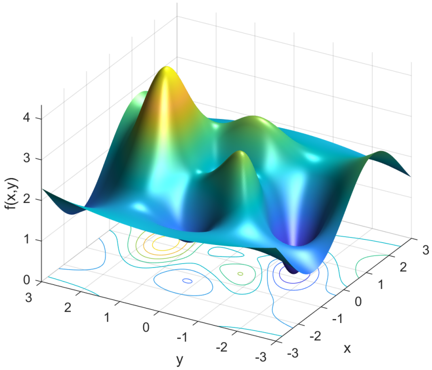

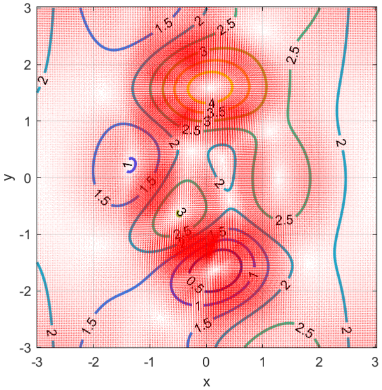

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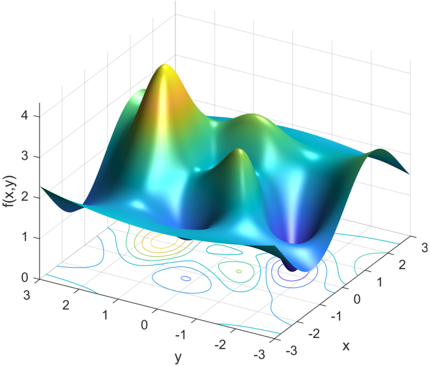

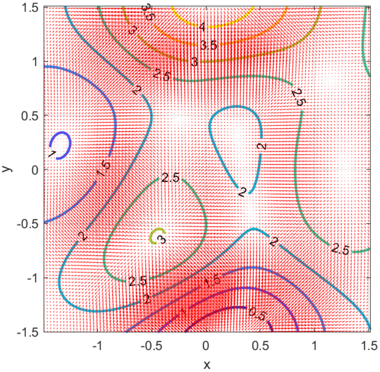

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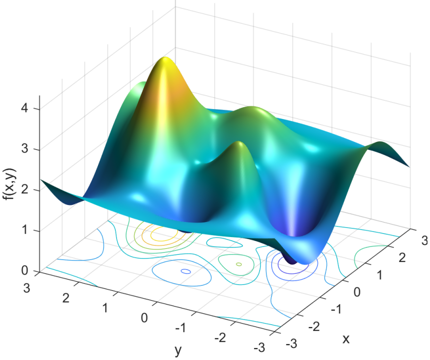

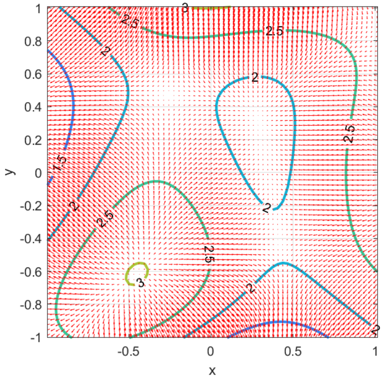

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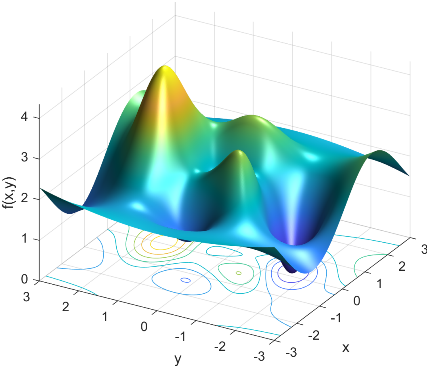

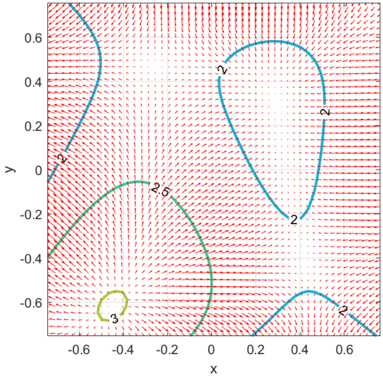

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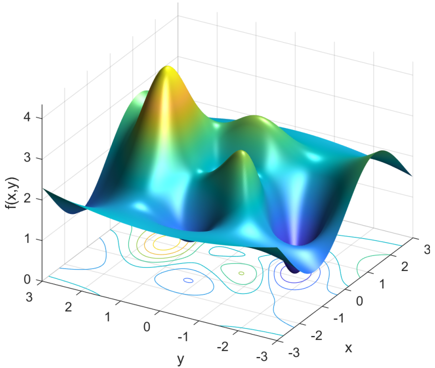

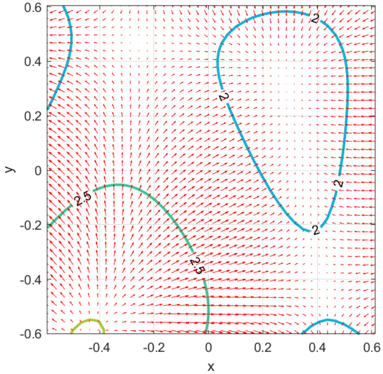

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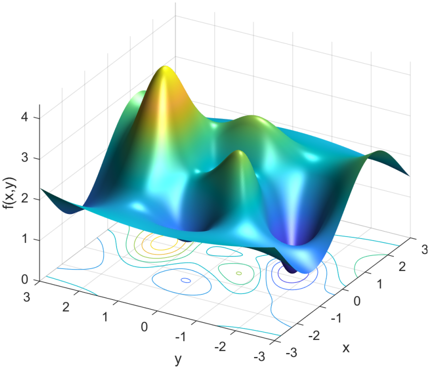
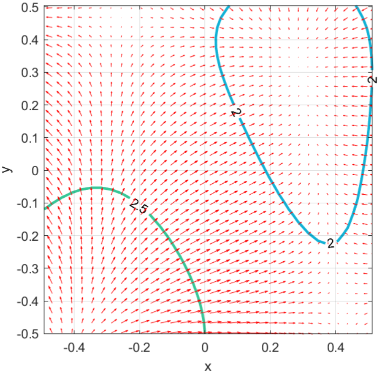
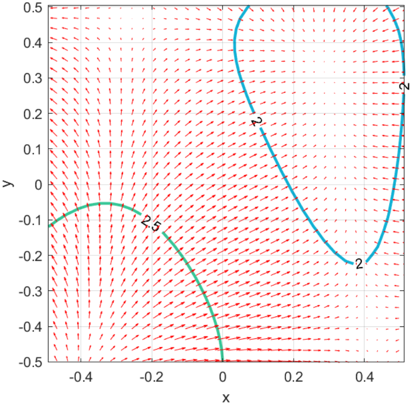




Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The gradient is orthogonal to level curves / level surfaces.



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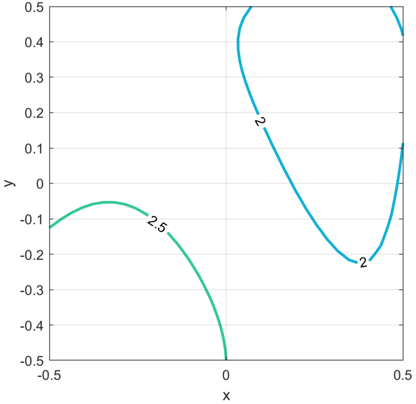

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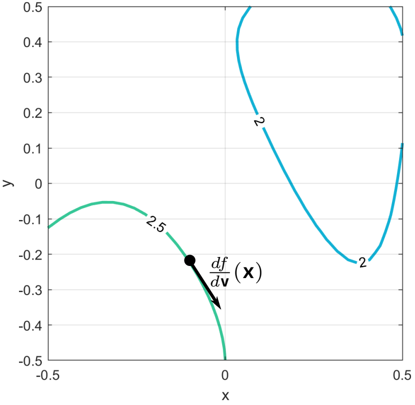

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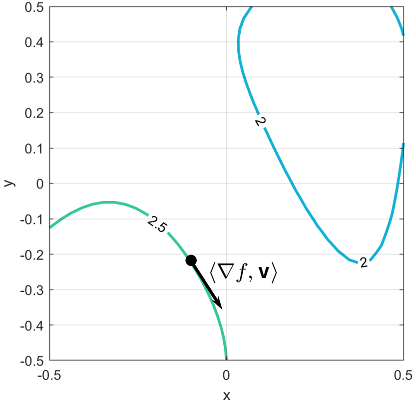

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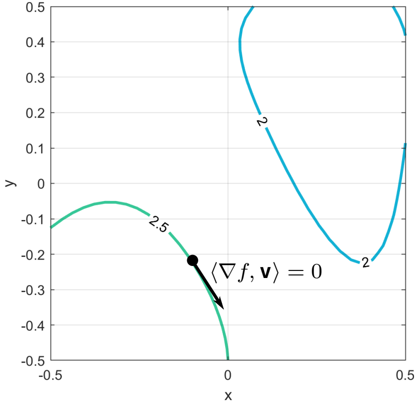

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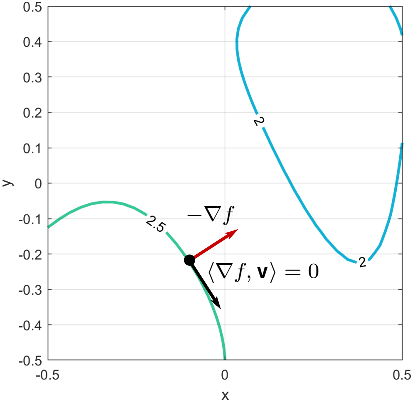

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See examples at: https://mathinsight.org/differentiability_multivariable_subtleties

Gradient descent: Stationary points

A stationary point is such that:

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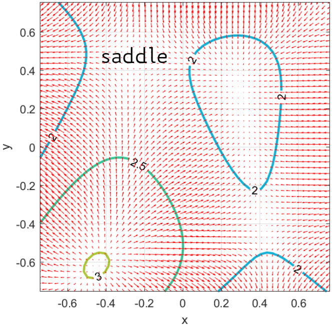

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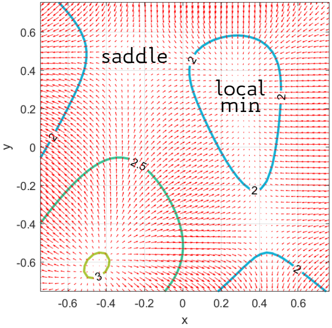

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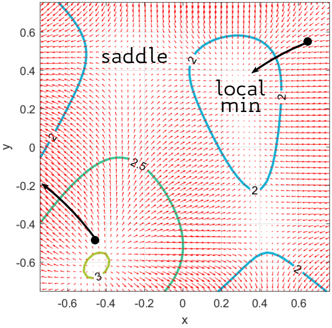
- Which stationary point depends on the initialization.



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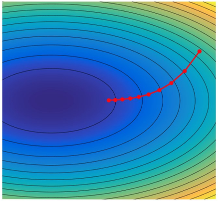

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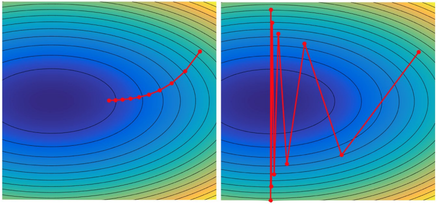

small α large α

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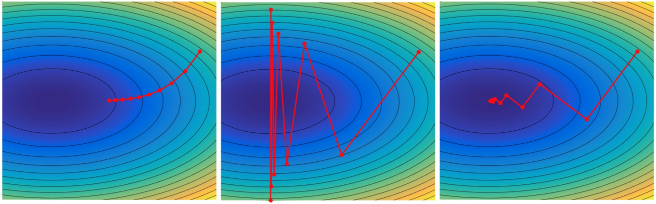
- Too small: slow convergence speed
- Too big: risk of overshooting
- Optimal values can be found via line search algorithms



small α | large α | optimal α

$\arg\min_\alpha f(\mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)}))$

Decay and momentum

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- Decrease α according to a decay parameter ρ:
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$$\mathbf{v}^{(t+1)} = \lambda \mathbf{v}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)}) \quad \text{momentum}$$
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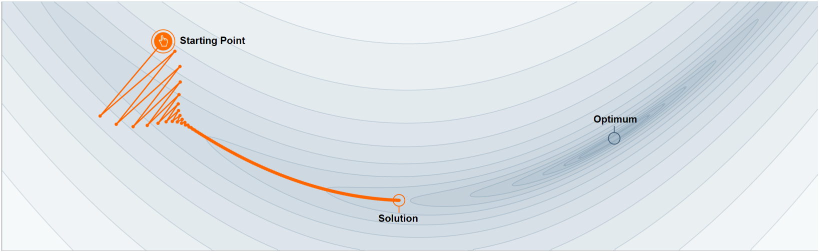
  Acceleration with big λ + escape from local minima.

Momentum



Goh, "Why momentum really works", Distill 2017

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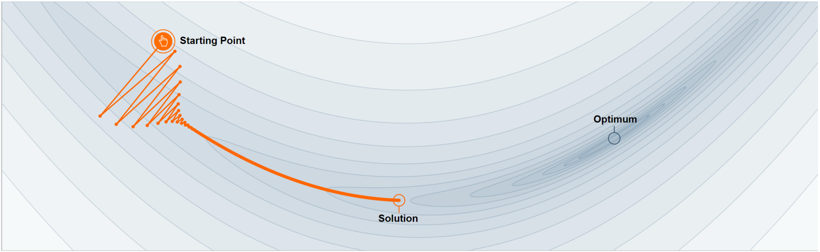

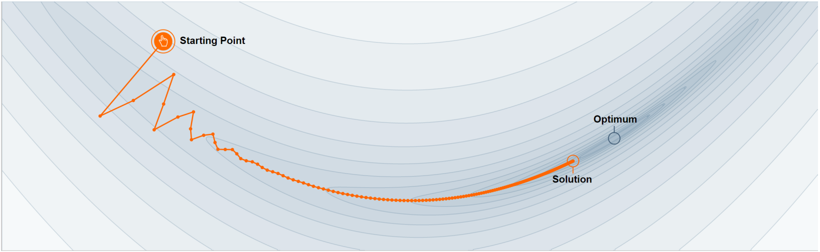

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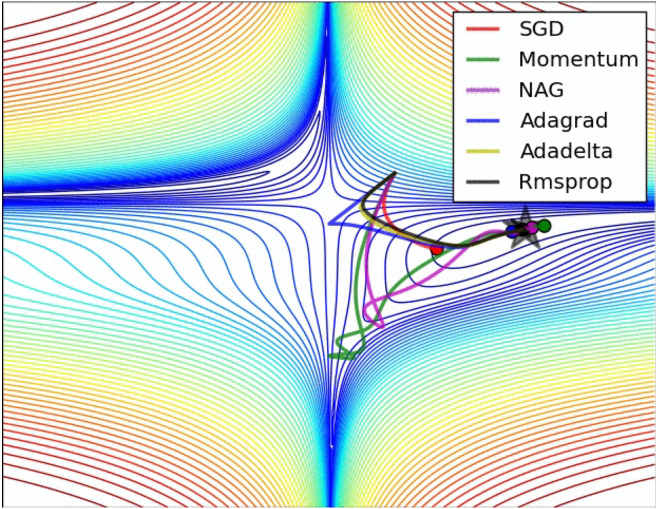
SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop

First-order acceleration methods

Let us try to unroll gradient descent:

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First-order acceleration methods

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&\vdots \\
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With momentum:

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The more general form:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(0)} + \alpha \sum_{i=0}^{t} \gamma_i^t \nabla f(\mathbf{x}^{(i)}) \quad \text{for some } \gamma_i$$

First-order acceleration methods

Let us try to unroll gradient descent:

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generalizes optimization algorithms like ADAM, AdaGrad, etc.

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Gradient descent for deep learning

In the general DL setting:

Each parameter gets updated so as to decrease the loss:

$$\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \alpha \frac{\partial \ell}{\partial \boldsymbol{\theta}_i}$$

The gradient tells us how to modify the parameters.

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- $\boldsymbol{\theta}$ stores the neural network params, possibly millions
- The loss may be non-convex and non-differentiable
- Be aware of computational aspects (e.g. $\nabla \|\mathbf{0}\|_1$?)

Stochastic gradient descent

Recall that the loss is defined over n training examples:

$$\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f_\Theta(x_i))^2$$

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Two bottlenecks make gradient descent impractical:

- Number of examples
- Number of parameters

Wilson and Martinez, "The general inefficiency of batch training for gradient descent learning", Neural Networks 2003

Mini-batches

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Compute $\nabla \ell_\Theta$ for a small representative subset of $m \ll n$ examples:

$$\frac{1}{m}\sum_{i=1}^{m} \nabla \hat{\ell}_\Theta(\mathcal{B}) \approx \frac{1}{n}\sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

The mini-batch $\mathcal{B} \subset \mathcal{T}$ is drawn uniformly.

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The true gradient $\nabla \ell_\Theta$ is approximated, but with a significant speed-up.

Example: MNIST dataset

$$n = 60,000\,,\;\; m = 10 \quad \Rightarrow \quad 6,000 \times \;\; \text{speedup}$$

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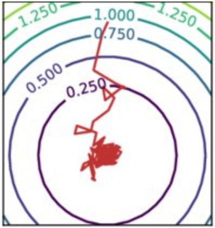
Remark: The update cost is constant regardless of $|\mathcal{T}|$!

Stochastic gradient descent



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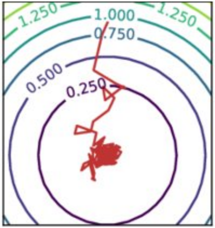

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Oscillations are due to the noise induced by the random sampling.

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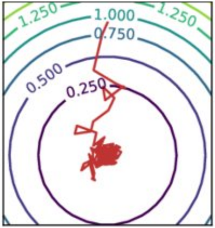

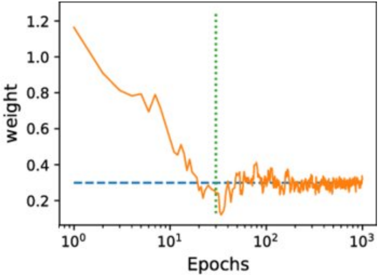

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Asymptotic upper bounds

For a convex problem, there is a true minimizer:

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$$|\underbrace{\ell(f_\Theta)}_{\text{GD/SGD}} - \underbrace{\ell(f^*)}_{\text{true}}| < \underbrace{\rho}_{\text{accuracy}}$$

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

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n training examples
d parameters
κ, ν are constants related to the conditioning of the problem

	cost per iteration	**iterations to reach** ρ
GD	$O(nd)$	$O(\kappa \log \frac{1}{\rho})$
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SGD does not depend on the number of examples, implying better generalization

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

Suggested reading

Distill article on why momentum really works:
https://distill.pub/2017/momentum/

Seminal paper on using mini-batches for training:
http://axon.cs.byu.edu/papers/Wilson.nn03.batch.pdf

Seminal paper on GD vs. SGD performance:
https://papers.nips.cc/paper/3323-the-tradeoffs-of-large-scale-learning.pdf