

Applied Machine Learning

Gradient Descent Methods

Reihaneh Rabbany



Learning objectives

Basic idea of

- gradient descent
- stochastic gradient descent
- method of momentum
- using an adaptive learning rate
- sub-gradient

Application to

- linear regression and classification

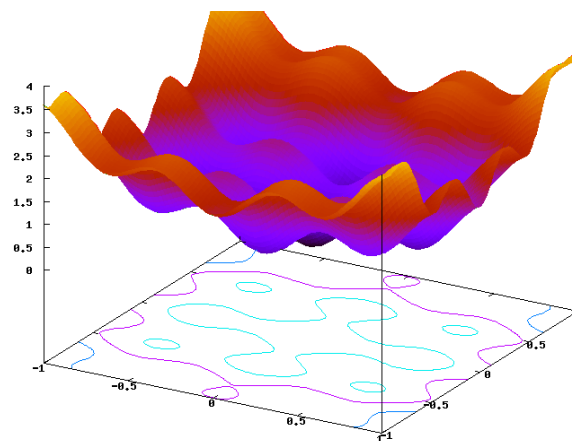
Optimization in ML

The core problem in ML is parameter estimation (aka model fitting), which requires solving **an optimization problem** of the loss/cost function

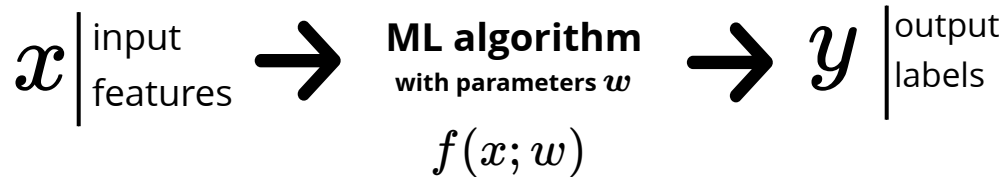
Optimization is a huge field

- discrete (combinatorial) vs **continuous variables**
- constrained vs **unconstrained**
- for continuous optimization in ML:
 - **convex** vs **non-convex**
 - looking for **local** vs global optima?
 - **analytic gradient**?
 - analytic Hessian?
 - **stochastic** vs **batch**
 - **smooth** vs non-smooth

bold marks
the settings
we consider
in this class



Optimization in ML



The core problem in ML is parameter estimation (aka model fitting), which requires solving **an optimization problem** of the loss/cost function

$$J(w) = \frac{1}{N} \sum_{n=1}^N l(y^{(n)}, f(x^{(n)}; w))$$

$$w^* = \arg \min_w J(w)$$

Recall

Linear Regression:

model:

$$\hat{y} = f_w(x) = w^\top x : \mathbb{R}^D \rightarrow \mathbb{R}$$

cost function:

$$J_w = \frac{1}{N} \sum_n \frac{1}{2} (y^{(n)} - \hat{y}^{(n)})^2$$

partial derivatives:

$$\frac{\partial}{\partial w_d} J_w = \frac{1}{N} \sum_n (\hat{y}^{(n)} - y^{(n)}) x_d^{(n)}$$

gradient: vector of all partial derivatives:

$$\nabla J(w) = \frac{1}{N} \sum_n (\hat{y}^{(n)} - y^{(n)}) x^{(n)}$$

$\text{D}x^1$

Logistic Regression:

$$\hat{y} = f_w(x) = \sigma(w^\top x) : \mathbb{R}^D \rightarrow \{0, 1\}$$

$$J_w = \frac{1}{N} \sum_n -y \log(\hat{y}^{(n)}) - (1 - y^{(n)}) \log(1 - \hat{y}^{(n)})$$

how to find w^*
given $\nabla J(w)$?

Gradient

Recall

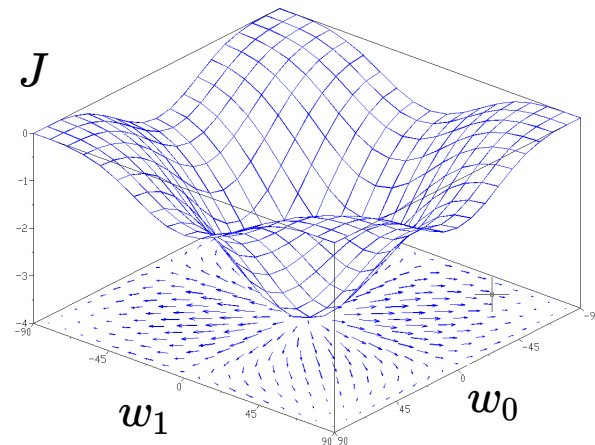
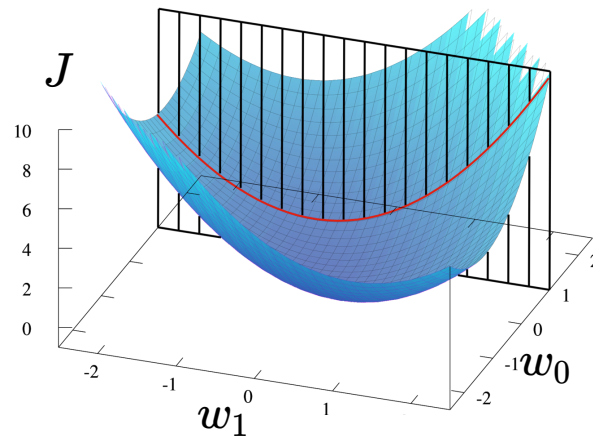
for a multivariate function $J(w_0, w_1)$
partial derivatives instead of derivative
= derivative when other vars. are fixed

$$\frac{\partial}{\partial w_1} J(w_0, w_1) \triangleq \lim_{\epsilon \rightarrow 0} \frac{J(w_0, w_1 + \epsilon) - J(w_0, w_1)}{\epsilon}$$

we can estimate this numerically if needed
(use small epsilon in the formula above)

gradient: vector of all partial derivatives

$$\nabla J(w) = \left[\frac{\partial}{\partial w_1} J(w), \dots, \frac{\partial}{\partial w_D} J(w) \right]^T$$



Gradient descent

an iterative algorithm for optimization

- starts from some $w^{\{0\}}$
- update using **gradient** $w^{\{t+1\}} \leftarrow w^{\{t\}} - \alpha \nabla J(w^{\{t\}})$
 - new notation!
 - steepest descent direction
 - learning rate
 - cost function
(for maximization : objective function)

converges to a local minima

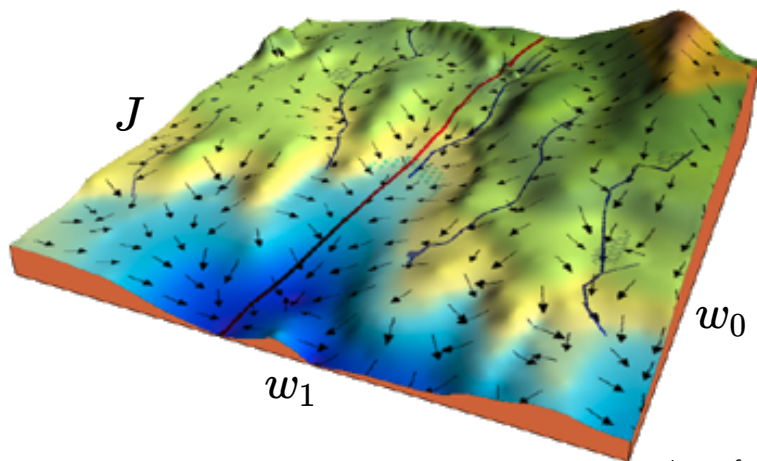
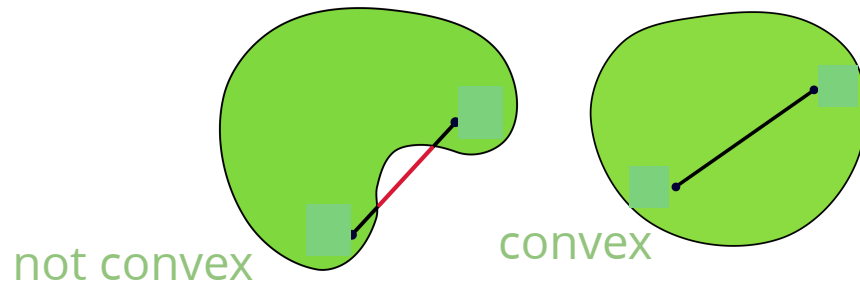


image from [here](#)

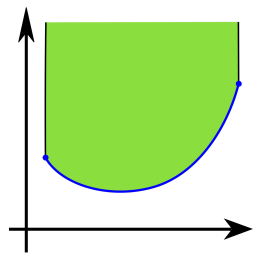
$$\nabla J(w) = \left[\frac{\partial}{\partial w_1} J(w), \dots, \frac{\partial}{\partial w_D} J(w) \right]^T$$

Convex function

a **convex** subset of $\mathbb{R}^N$ intersects any line in at most one line segment

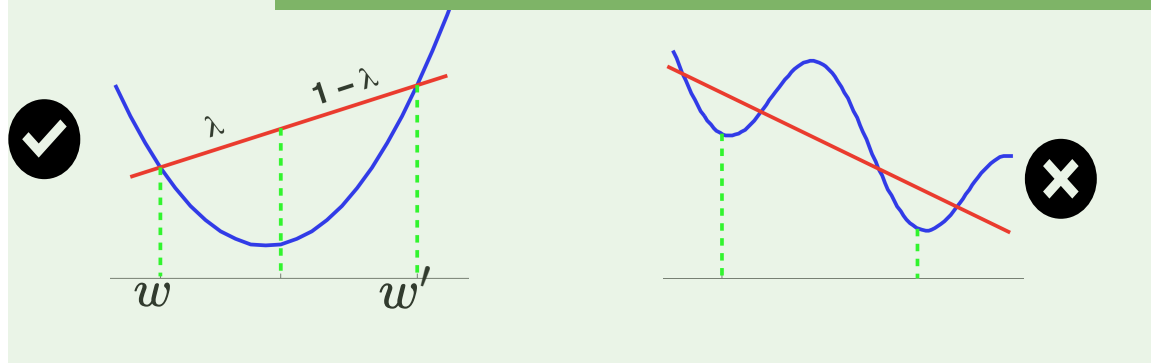


a **convex function** is a function for which the *epigraph* is a **convex set**



epigraph: set of all points above the graph

$$f(\lambda w + (1 - \lambda)w') \leq \lambda f(w) + (1 - \lambda)f(w') \quad 0 < \lambda < 1$$



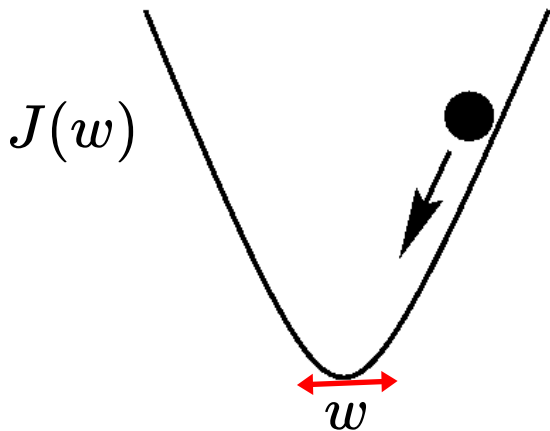
Minimum of a convex function

Convex functions are easier to minimize:

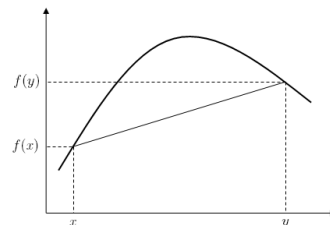
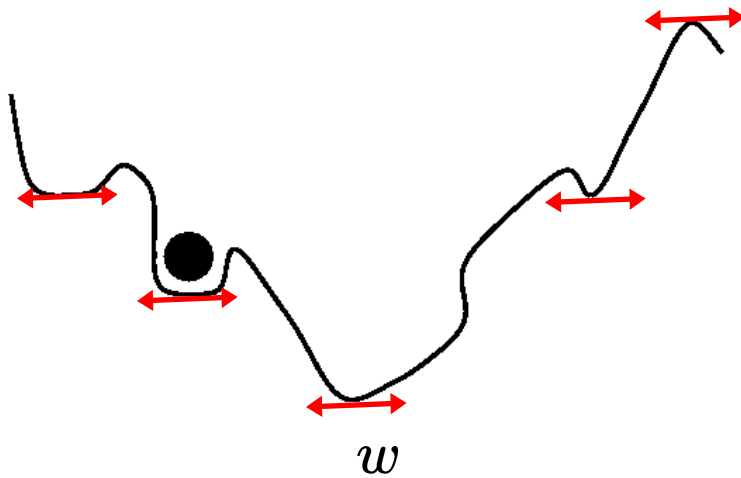
- critical points are global minimum
- gradient descent can find it

$$w^{\{t+1\}} \leftarrow w^{\{t\}} - \alpha \nabla J(w^{\{t\}})$$

convex



non-convex: gradient descent may find a local optima



a **concave** function is a negative of a convex function (easy to **maximize**)

Recognizing convex functions

a constant function is convex $f(x) = c$

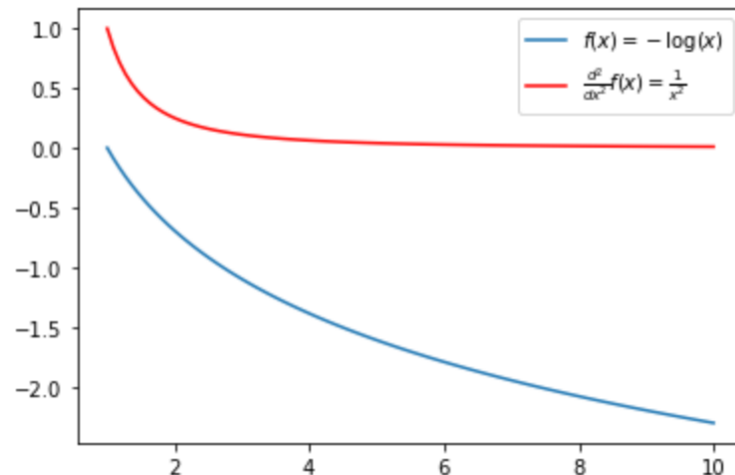
a linear function is convex $f(x) = w^\top x$

convex if second derivative is positive everywhere $\frac{d^2}{dx^2} f \geq 0 \quad \forall x$

examples $x^{2d}, e^{ax}, -\log(x), -\sqrt{x}$

$x \log(x), x > 0$

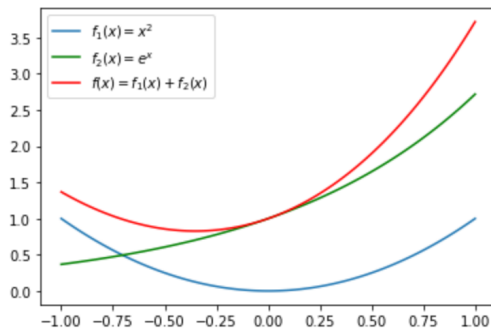
$x^a, x > 0, a > 1$



Recognizing convex functions

sum of convex functions is convex

example 1:



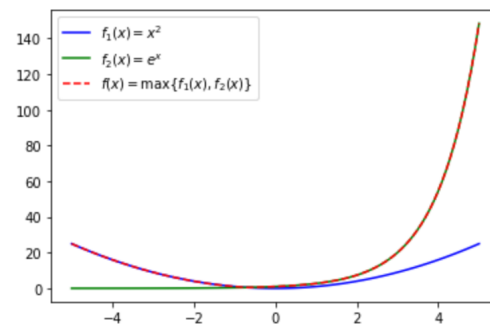
example 2:

sum of squared errors

$$J(w) = \|Xw - y\|_2^2 = \sum_n (w^\top x^{(n)} - y)^2$$

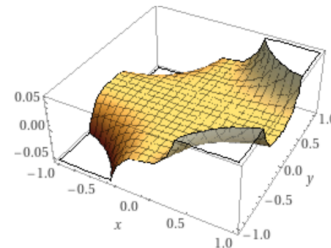
maximum of convex functions is convex

example 1:



example 2:

$$f(y) = \max_{x \in [0,2]} x^3 y^4 = 8y^4$$



note this is not convex in x 10

Recognizing convex functions

composition of convex functions is generally **not** convex

example

$$(-\log(x))^2$$

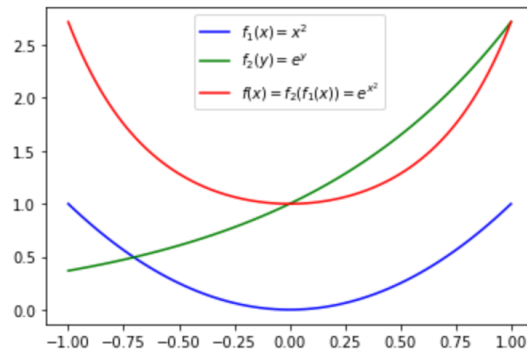
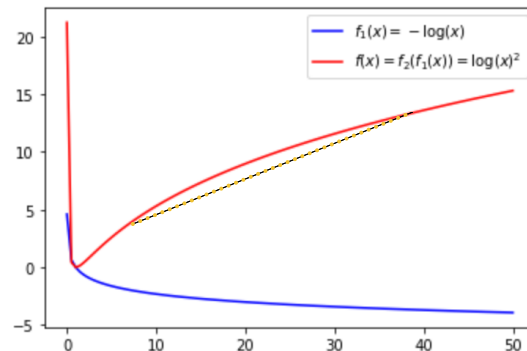
however, if f , g are convex, and g is **non-decreasing**,
then $g(f(x))$ is convex

example

$$e^{f(x)}$$

for convex f

Composition with affine map (linear function) is also convex, e.g. $f(w^\top x - y)$ if f is convex



Recognizing convex functions

is the logistic regression cost function convex in model parameters (w)?

$$J(w) = \frac{1}{N} \sum_{n=1}^N y^{(n)} \log(1 + e^{-w^\top x}) + (1 - y^{(n)}) \log(1 + e^{w^\top x})$$

Annotations:

- non-negative
- linear
- same argument
- checking second derivative
- sum of convex functions

$$\frac{\partial^2}{\partial z^2} \log(1 + e^z) = \frac{e^{-z}}{(1+e^{-z})^2} \geq 0$$

Gradient Descent

implementing gradient descent is easy!



```
1 def GradientDescent(x, # N x D
2                     y, # N
3                     lr=.01, # learning rate
4                     eps=1e-2, # termination condition
5                     ):
6     N,D = x.shape
7     w = np.zeros(D)
8     g = np.inf
9     while np.linalg.norm(g) > eps:
10         g = gradient(x, y, w)
11         w = w - lr*g
12     return w
13
```

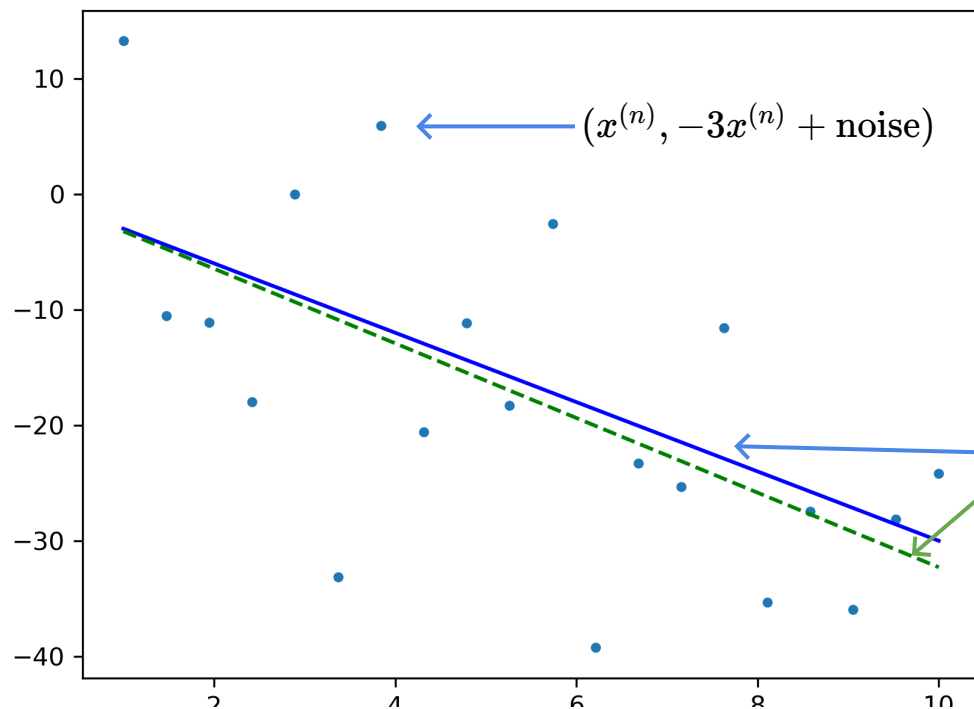
code on the previous page

Some termination condition:

- some max #iterations
- small gradient
- a small change in the objective
- increasing error on validation set

early stopping (one way to avoid overfitting) 14

example GD for linear regression



using direct solution method
 $w = (X^T X)^{-1} X^T y \approx -3.2$

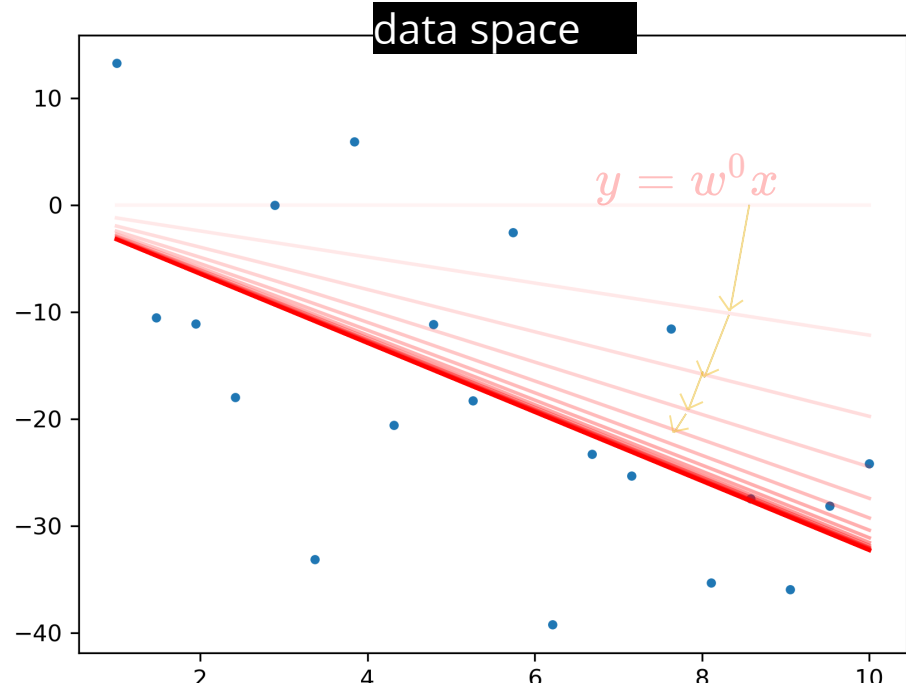
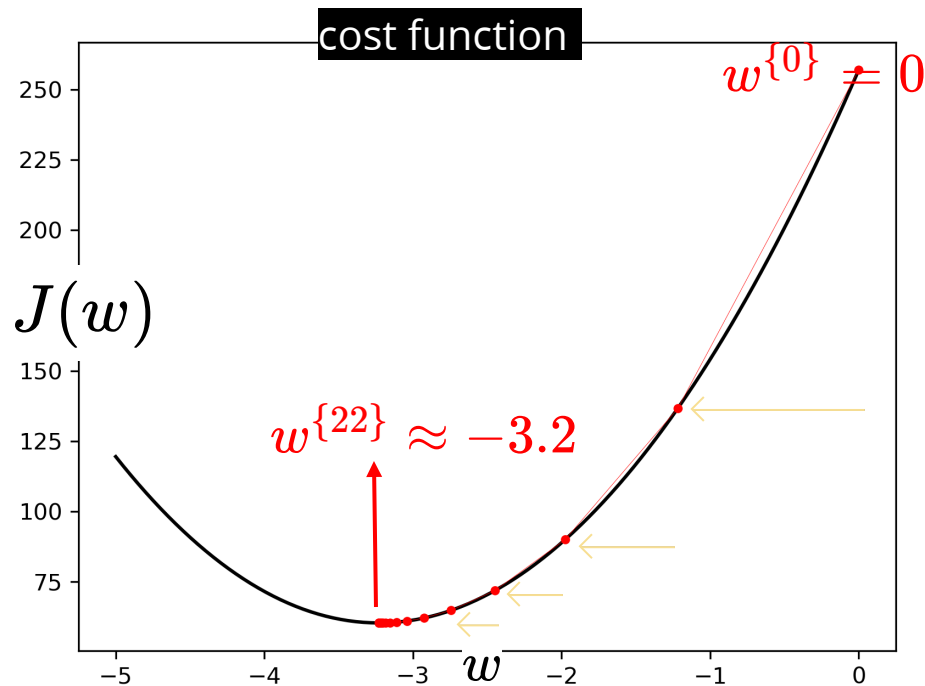
$$y = wx$$

$$y = -3x$$

example

GD for linear regression

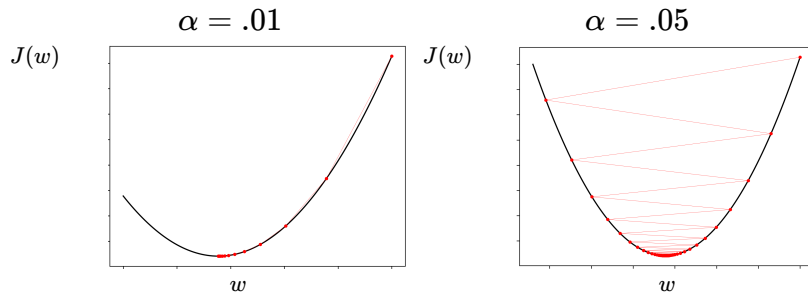
After 22 steps $w^{\{t+1\}} \leftarrow w^{\{t\}} - .01 \nabla J(w^{\{t\}})$



Learning rate α

Learning rate has a significant effect on GD

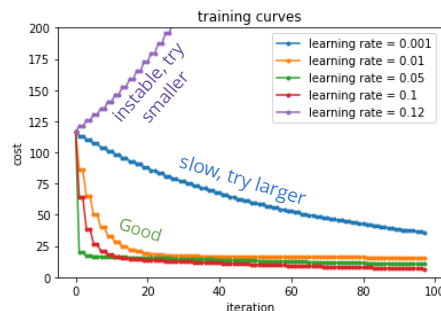
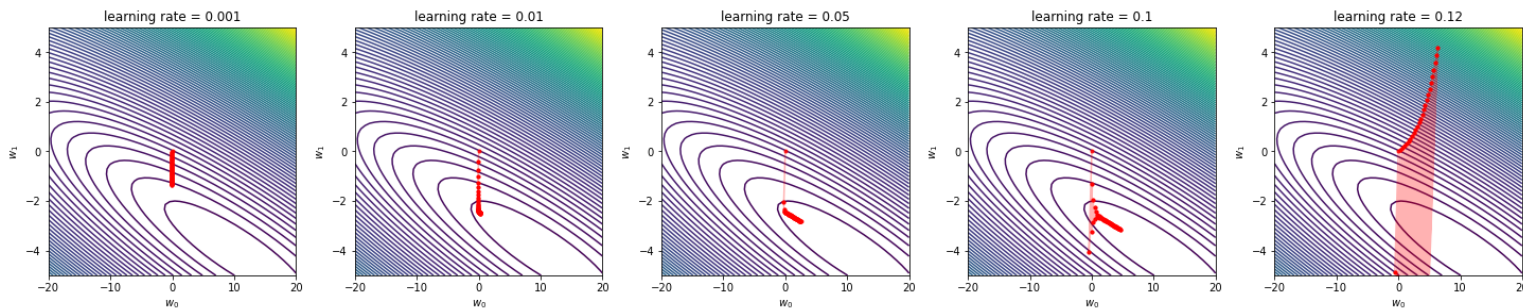
example, $D=1$
linear regression



too **small**: may take a long time to converge

too **large**: it overshoots or even diverges

example, $D=2$
linear regression
50 gradient steps



do a grid search usually between 0.001 to .1 to find the right value, look at the training curves

Stochastic Gradient Descent

we can write the cost function as an average over instances

$$J(w) = \frac{1}{N} \sum_{n=1}^N J_n(w)$$

cost for a single data-point
e.g. for linear regression

$$J_n(w) = \frac{1}{2} (w^T x^{(n)} - y^{(n)})^2$$

the same is true for the partial derivatives

$$\frac{\partial}{\partial w_j} J(w) = \frac{1}{N} \sum_{n=1}^N \frac{\partial}{\partial w_j} J_n(w)$$

therefore $\nabla J(w) = \mathbb{E}_{\mathcal{D}} [\nabla J_n(w)]$

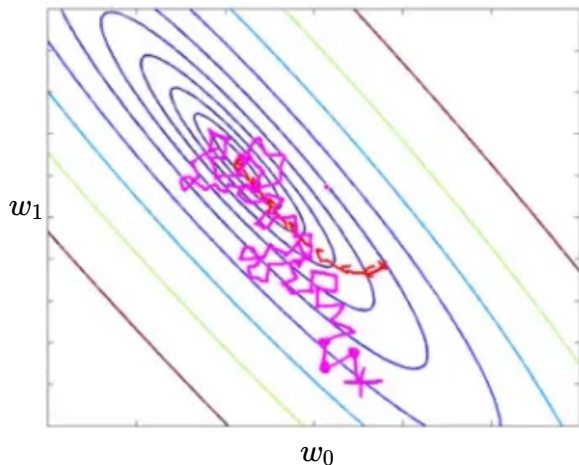
Stochastic Gradient Descent

Idea: use stochastic approximations $\nabla J_n(w)$ in gradient descent

stochastic gradient update

$$w \leftarrow w - \alpha \nabla J_n(w)$$

the steps are "on average" in the right direction



each step is using gradient of a different cost, $J_n(w)$

each update is $(1/N)$ of the cost of batch gradient

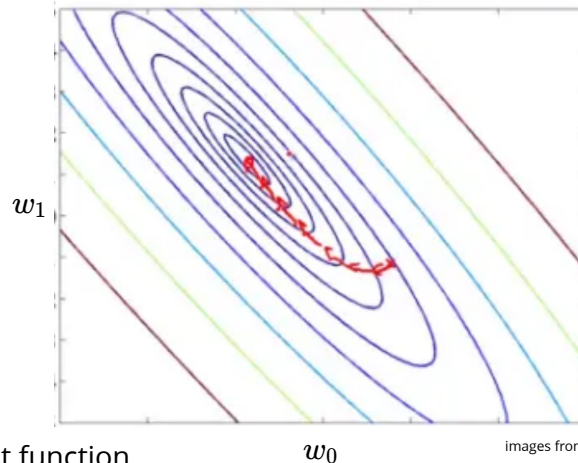
e.g., for linear regression $\mathcal{O}(D)$

$$\nabla J_n(w) = x^{(n)}(w^\top x^{(n)} - y^{(n)})$$

batch gradient update

$$w \leftarrow w - \alpha \nabla J(w)$$

with small learning rate: guaranteed improvement at each step



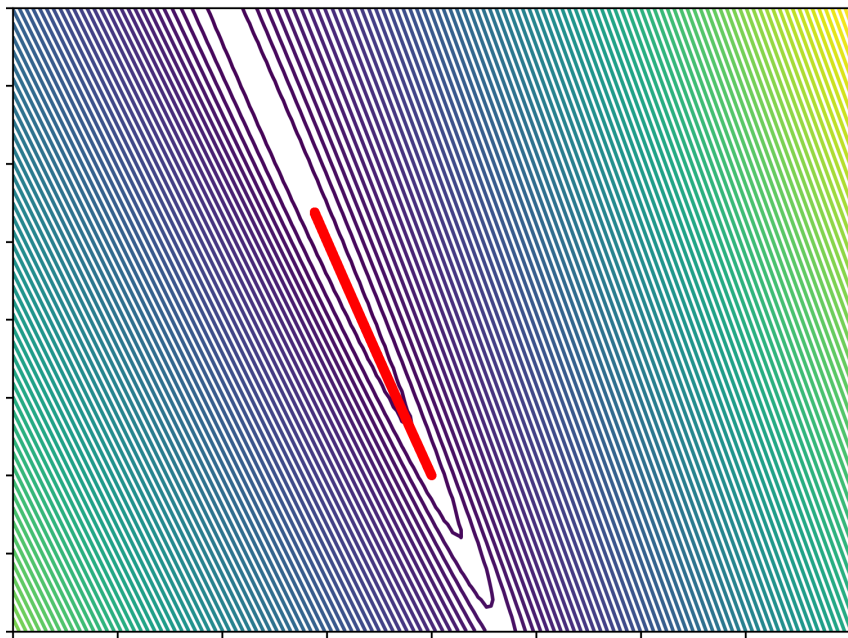
contour plot of the cost function

images from [here](#)

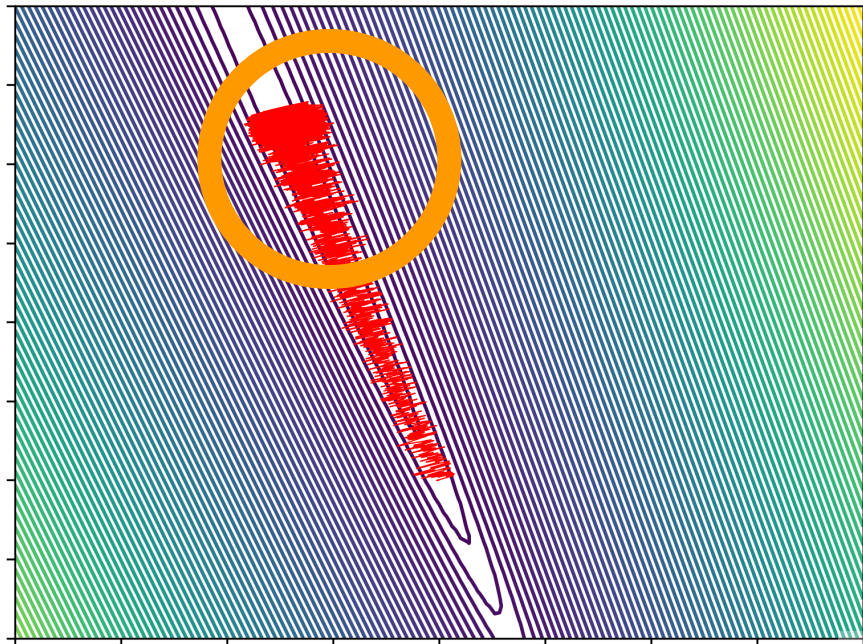
SGD for logistic regression example

logistic regression for Iris dataset ($D=2$, $\alpha = .1$)

batch gradient



stochastic gradient



Convergence of SGD

stochastic gradients are not zero even at the optimum w
how to guarantee convergence?

idea: **schedule** to have a smaller learning rate over time

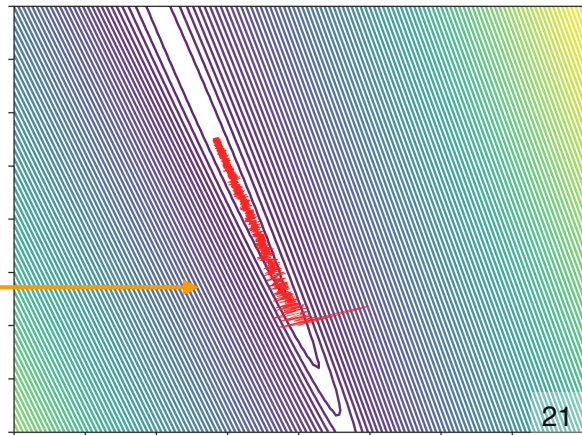
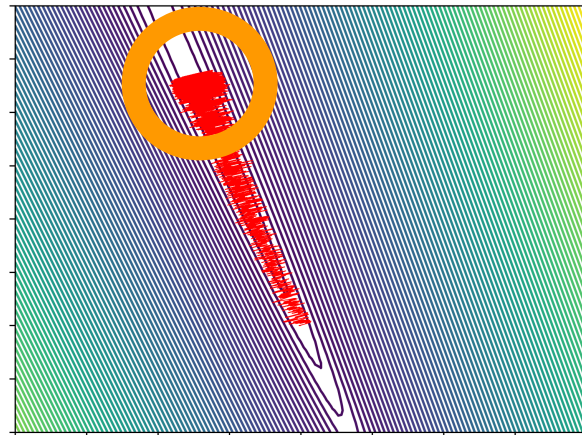
Robbins Monro

the sequence we use should satisfy: $\sum_{t=0}^{\infty} \alpha^{\{t\}} = \infty$

& otherwise for large $\|w^{\{0\}} - w^*\|$ we can't reach the minimum

the steps should go to zero $\sum_{t=0}^{\infty} (\alpha^{\{t\}})^2 < \infty$

example $\alpha^{\{t\}} = \frac{10}{t}, \alpha^{\{t\}} = t^{-.51}$



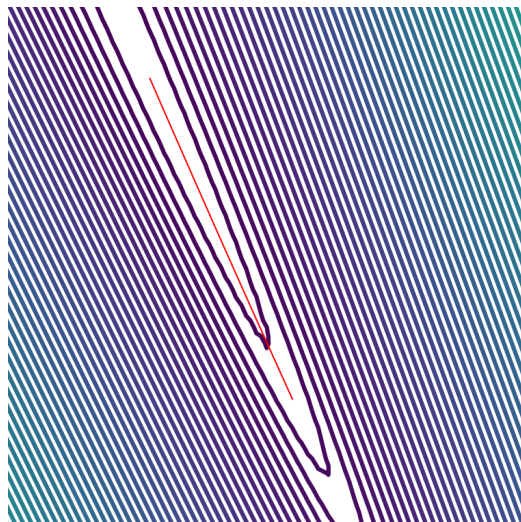
Minibatch SGD

use a minibatch to produce gradient estimates

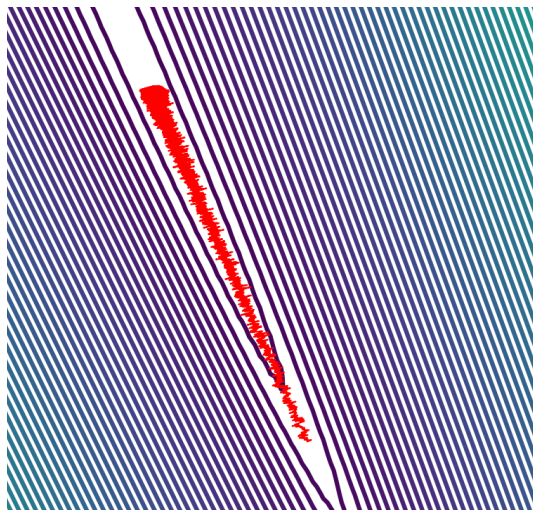
$$\nabla J_{\mathbb{B}} = \frac{1}{|\mathbb{B}|} \sum_{n \in \mathbb{B}} \nabla J_n(w)$$

$\mathbb{B} \subseteq \{1, \dots, N\}$ a subset of the dataset

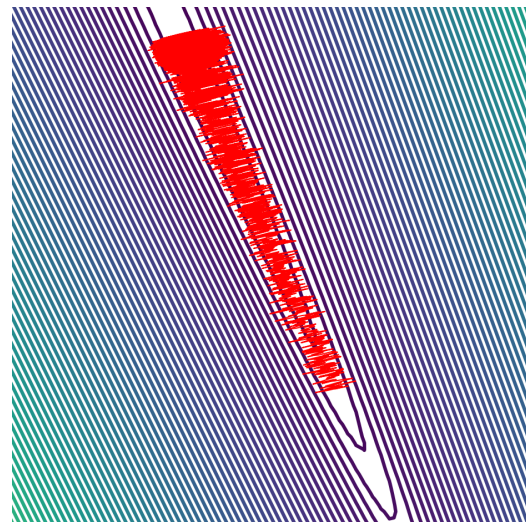
GD full batch



SGD minibatch-size=16

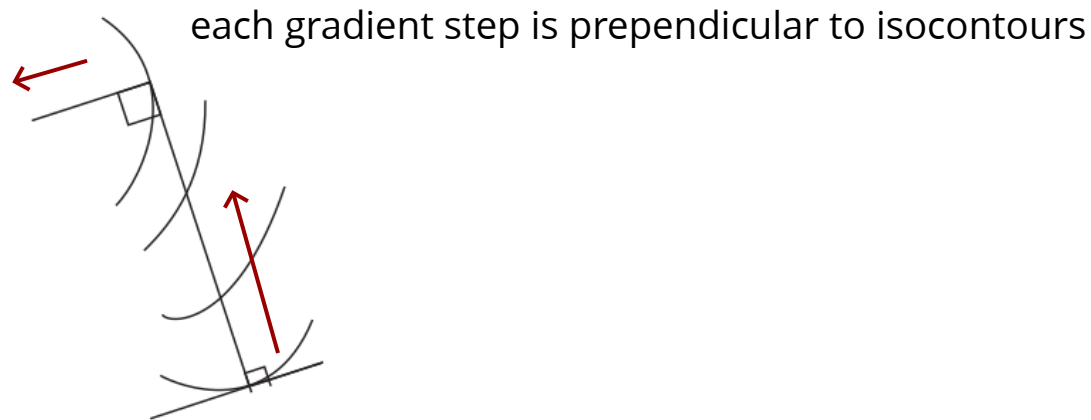
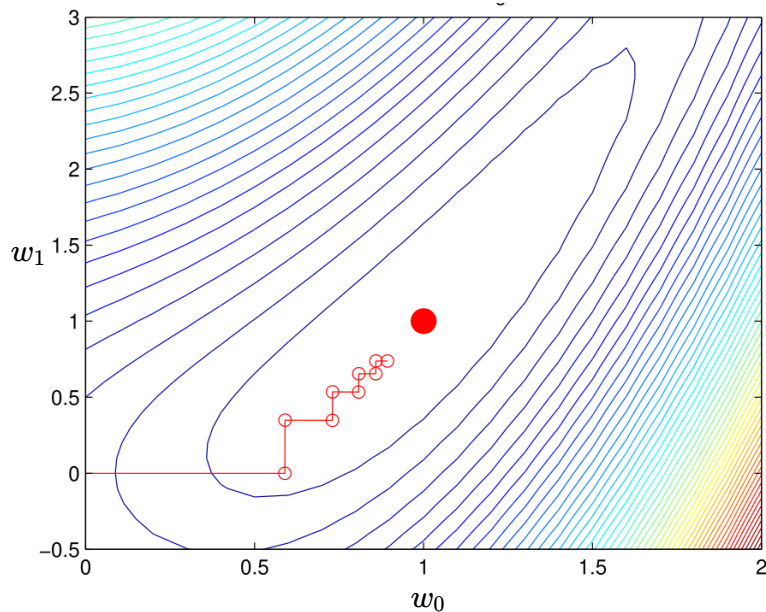


SGD minibatch-size=1



Oscillations

gradient descent can oscillate a lot!



in SGD this is worsened due to *noisy* gradient estimate

Momentum

to help with oscillations:

- use a **running average** of gradients
- more recent gradients should have higher weights

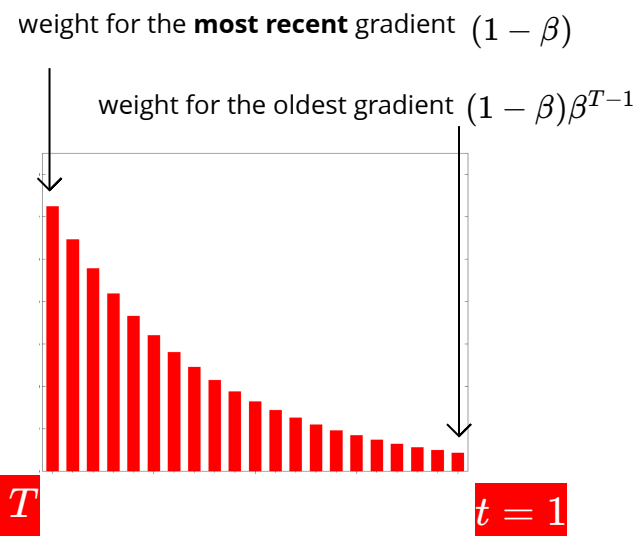
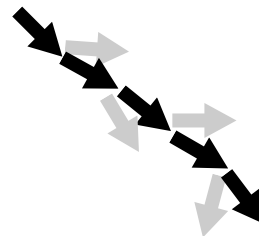
$$\Delta w^{\{t\}} \leftarrow \beta \Delta w^{\{t-1\}} + (1 - \beta) \nabla J_{\mathbb{B}}(w^{\{t-1\}})$$
$$w^{\{t\}} \leftarrow w^{\{t-1\}} - \alpha \Delta w^{\{t\}}$$

| momentum of 0 reduces to SGD
common value > .9

is effectively an **exponential moving average**

$$\Delta w^{\{T\}} = \sum_{t=1}^T \beta^{T-t} (1 - \beta) \nabla J_{\mathbb{B}}(w^{\{t\}})$$

there are other variations of momentum with similar idea

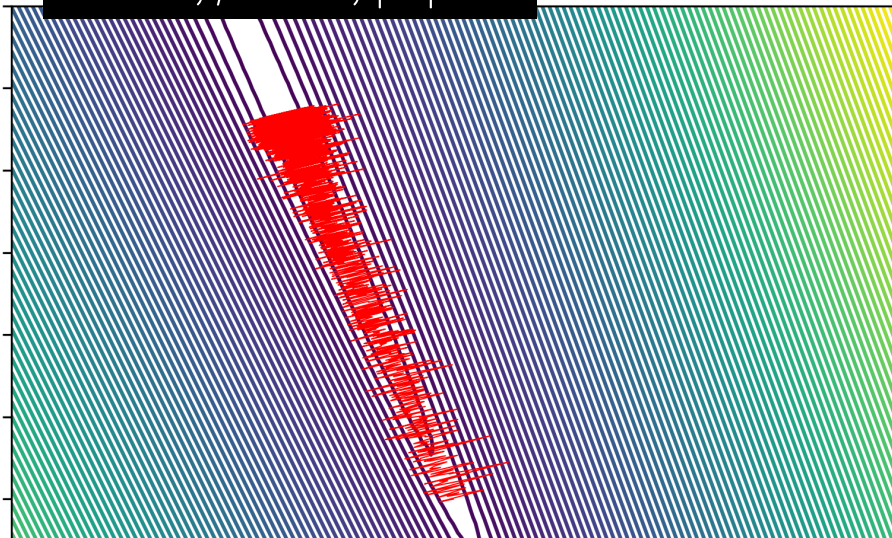


Momentum

Example: logistic regression

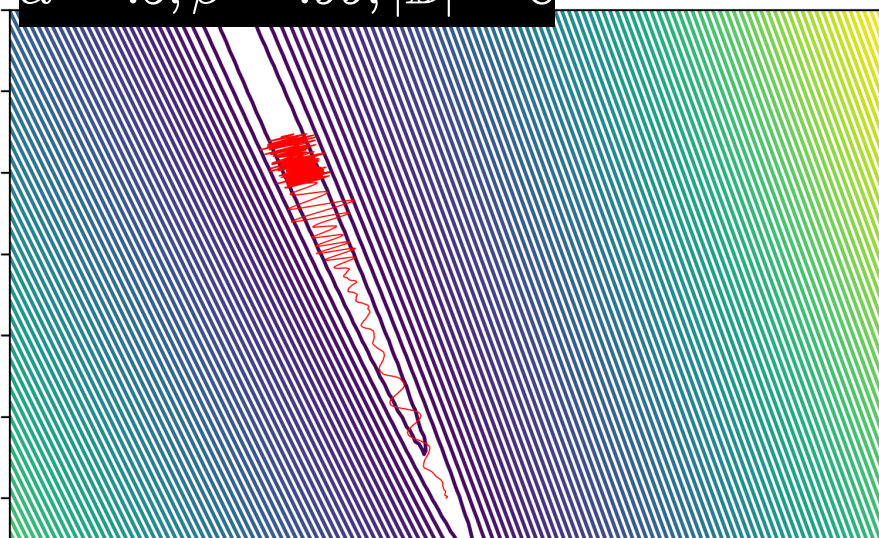
no momentum

$$\alpha = .5, \beta = 0, |\mathbb{B}| = 8$$



with momentum

$$\alpha = .5, \beta = .99, |\mathbb{B}| = 8$$



see the beautiful demo at Distill <https://distill.pub/2017/momentum/>

Adagrad (Adaptive gradient)

use different learning rate for each parameter w_d

also make the learning rate **adaptive**

$$S_d^{\{t\}} \leftarrow S_d^{\{t-1\}} + \frac{\partial}{\partial w_d} J(w^{\{t-1\}})^2$$

sum of squares of derivatives over all iterations so far (for individual parameter)

$$w_d^{\{t\}} \leftarrow w_d^{\{t-1\}} - \frac{\alpha}{\sqrt{S_d^{\{t\}} + \epsilon}} \frac{\partial}{\partial w_d} J(w^{\{t-1\}})$$

the learning rate is adapted to previous updates

ϵ is to avoid numerical issues

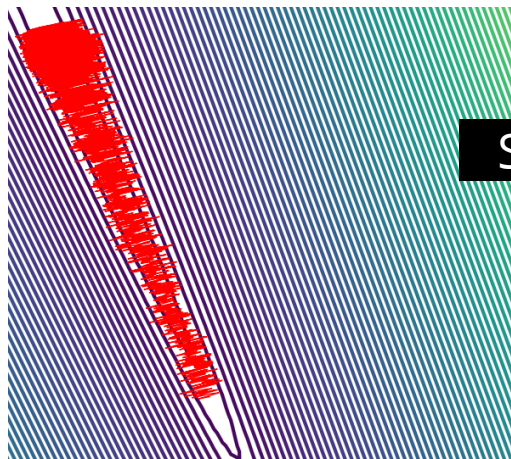
useful when parameters are updated at different rates

(e.g., sparse data when some features are often zero when using SGD)

Adagrad (Adaptive gradient)

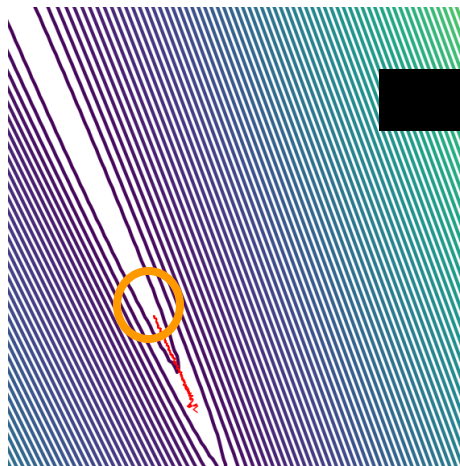
different learning rate for each parameter w_d
make the learning rate adaptive

$\alpha = .1, |\mathbb{B}| = 1, T = 80,000$



SGD

$\alpha = .1, |\mathbb{B}| = 1, T = 80,000, \epsilon = 1e-8$



Adagrad

problem: the learning rate goes to zero too quickly

RMSprop (Root Mean Squared propagation)

solve the problem of diminishing step-size with Adagrad

- use **exponential moving average** instead of sum (similar to momentum)

instead of Adagrad: $S_d^{\{t\}} \leftarrow S_d^{\{t-1\}} + \frac{\partial}{\partial w_d} J(w^{\{t-1\}})^2$

$$S^{\{t\}} \leftarrow \gamma S^{\{t-1\}} + (1 - \gamma) \nabla J(w^{\{t-1\}})^2$$

$$w^{\{t\}} \leftarrow w_{\{t-1\}} - \frac{\alpha}{\sqrt{S^{\{t\}} + \epsilon}} \nabla J(w^{\{t-1\}})$$

identical to Adagrad

note that $S^{\{t\}}$ here is a vector and with the square root is element-wise

the default algorithm in practice

Adam (Adaptive Moment Estimation)

two ideas so far:

1. use momentum to smooth out the oscillations
2. adaptive per-parameter learning rate

both use exponential moving averages

Adam **combines the two**:

$$\begin{aligned} M^{\{t\}} &\leftarrow \beta_1 M^{\{t-1\}} + (1 - \beta_1) \nabla J(w^{\{t-1\}}) && \text{identical to method of momentum} \\ &&& \text{(moving average of the first moment)} \\ S^{\{t\}} &\leftarrow \beta_2 S^{\{t-1\}} + (1 - \beta_2) \nabla J(w^{\{t-1\}})^2 && \text{identical to RMSProp} \\ &&& \text{(moving average of the second moment)} \\ w^{\{t\}} &\leftarrow w^{\{t-1\}} - \frac{\alpha}{\sqrt{\hat{S}^{\{t\}} + \epsilon}} \hat{M}^{\{t\}} \end{aligned}$$

since M and S are initialized to be zero, at early stages they are biased towards zero

$$\hat{M}^{\{t\}} \leftarrow \frac{M^{\{t\}}}{1 - \beta_1^t}$$

$$\hat{S}^{\{t\}} \leftarrow \frac{S^{\{t\}}}{1 - \beta_2^t}$$

for large time-steps it has no effect
for small t, it scales up numerator

In practice

the list of methods is growing ...

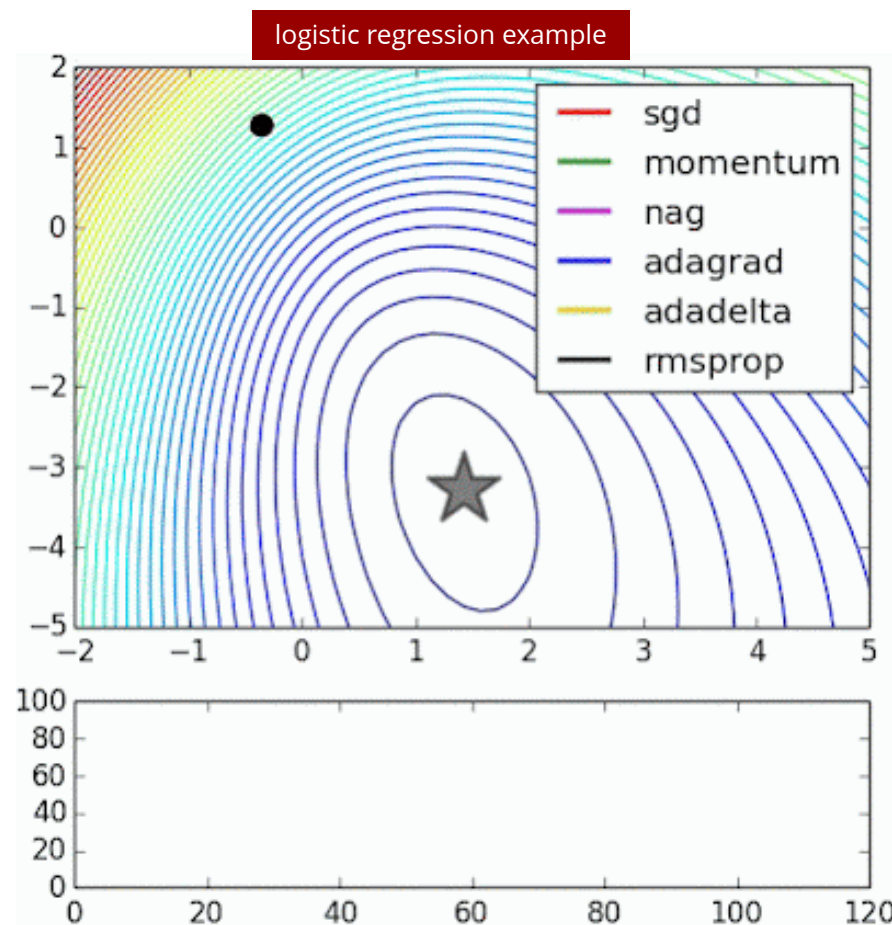
they have recommended range of parameters

- *learning rate, momentum etc.*

still may need some hyper-parameter tuning

these are all **first order methods**

- they only need the first derivative
- 2nd order methods can be much more effective, but also much more expensive



Summary

learning: optimizing the model parameters (minimizing a cost function)

use **gradient descent** to find local minimum

- easy to implement (esp. using automated differentiation)
- for **convex functions** gives global minimum

Stochastic GD: for large data-sets use mini-batch for a noisy-fast estimate of gradient

- **Robbins Monro** condition: reduce the learning rate to help with the noise

better (stochastic) gradient optimization

- **Momentum:** exponential running average to help with the noise
- **Adagrad & RMSProp:** per parameter adaptive learning rate
- **Adam:** combining these two ideas