Applied Machine Learning

Gradient Descent Methods

Siamak Ravanbakhsh

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Learning objectives

Basic idea of

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

Application to

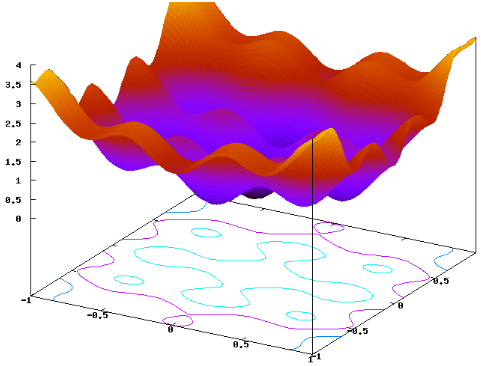
- linear regression and classification

Optimization in ML

Inference and learning of a model often involves optimization:

optimization is a huge field

bold: the setting considered in this class



- 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

Gradient

for a multivariate function $J(w_0, w_1)$

partial derivatives instead of derivative

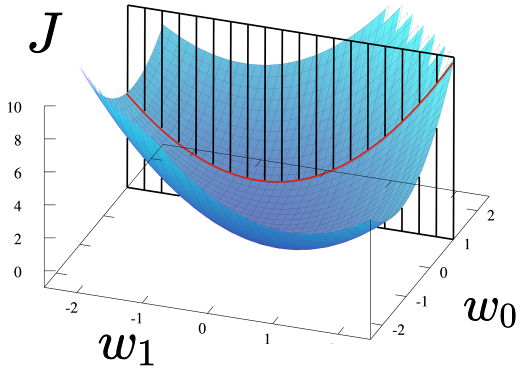
= derivative when other vars. are fixed

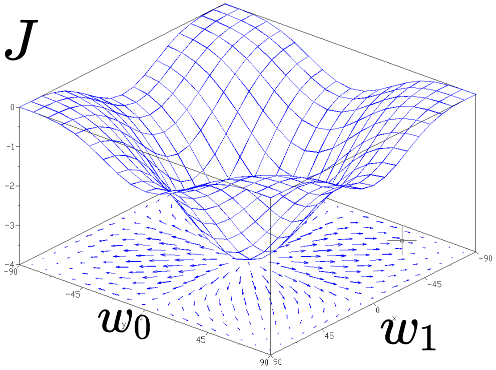
$$\frac{\partial}{\partial w_1} J(w_0, w_1) \triangleq \lim_{\epsilon \to 0} \frac{J(w_0, w_1 + \epsilon) - J(w_0, w_1)}{\epsilon}$$

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

gradient: vector of all partial derivatives

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





Gradient descent

an iterative algorithm for optimization

- starts from some $w^{\{0\}}$
- update using gradient $w^{\{t+1\}} \leftarrow w^{\{t\}} - \alpha \nabla \mathcal{J}(w^{\{t\}})$

steepest descent direction

learning rate

cost function

(for maximization : objective function)

$$\nabla \mathcal{J}(w) = [\frac{\partial}{\partial w_1}\mathcal{J}(w), \cdots \frac{\partial}{\partial w_D}\mathcal{J}(w)]^T$$

converges to a local minima

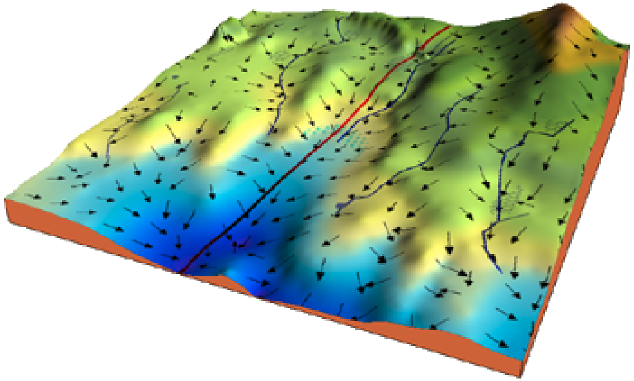
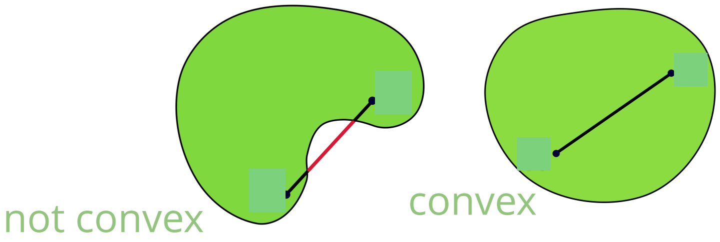


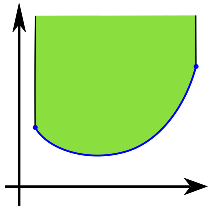
image: https://ml-cheatsheet.readthedocs.io/en/latest/gradient_descent.html

Convex function

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

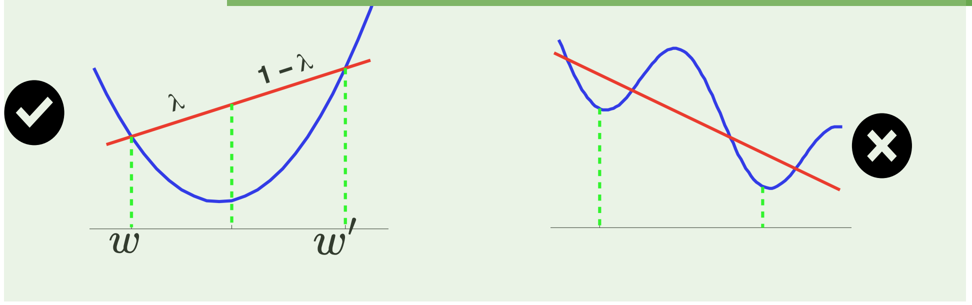


a **convex function** is a function for which the *epigraph* is a **convex set**



epigraph: set of all points above the graph

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

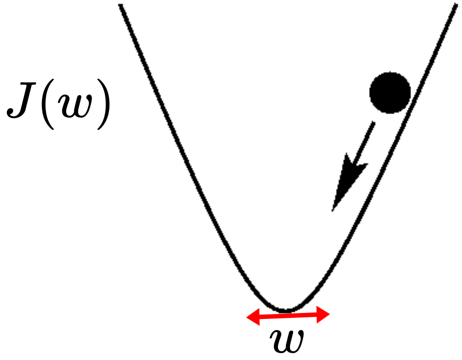


Convex function

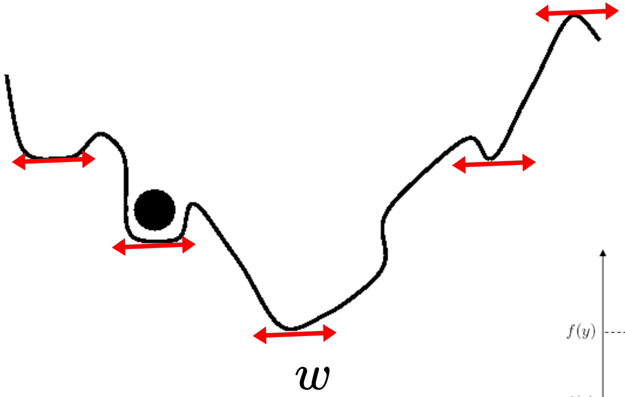
Convex functions are easier to minimize:

- critical points are global minimum
- gradient descent can find it $w^{\{t+1\}} \leftarrow w^{\{t\}} - \alpha \nabla \mathcal{J}(w^{\{t\}})$

convex



non-convex: gradient descent may find a local optima



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

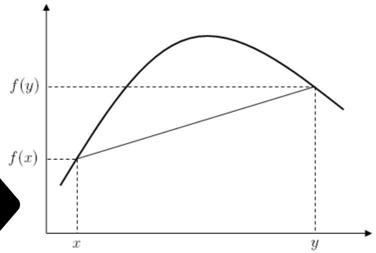


image: https://www.willamette.edu/~gorr/classes/cs449/momrate.html

Recognizing convex functions

a linear function is convex $w^T x$

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

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

sum of convex functions is convex example $||WX - Y||_2^2 + \lambda ||w||_2^2$

maximum of convex functions is convex example $f(y) = \max_{x \in [1,5]} \sqrt{x} y^4$

note this is not convex in x

composition of convex functions is generally **not** convex example $(-\log(x))^2$

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

example $e^{f(x)}$

for convex ***f***

Gradient for linear and logistic regression

in both cases: $\nabla J(w) = \overset{D \times N}{X^T} \overset{N \times 1}{(\hat{y} - y)}$

linear regression: $\hat{y} = \overset{N \times D}{X} \overset{D \times 1}{w}$

logistic regression: $\hat{y} = \sigma(Xw)$

```python
def gradient(X, y, w):
    N,D = X.shape
    yh = logistic(np.dot(X, w))
    grad = np.dot(X.T, yh - y) / N
    return grad
```

time complexity: $\mathcal{O}(ND)$

(two matrix multiplications)

compared to the direct solution for linear regression: $\mathcal{O}(ND^2 + D^3)$

gradient descent can be much faster for large D

Gradient Descent

implementing gradient descent is easy!

```
def GradientDescent(X, # N x D
                    y, # N
                    lr=.01, # learning rate
                    eps=1e-2, # termination codition
                   ):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    while np.linalg.norm(g) > eps:
        g = gradient(X, y, w)
        w = w - lr*g
    return w

```

code on the previous page

Some **termination conditions**:

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

early stopping (one way to avoid overfitting)

Example: GD for Linear Regression

applying this to to fit toy data

```
def GradientDescent(X, # N x D
                    y, # N
                    lr=.01, # learning rate
                    eps=1e-2, # termination codition
                   ):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    while np.linalg.norm(g) > eps:
        g = gradient(X, y, w)
        w = w - lr*g
    return w

```

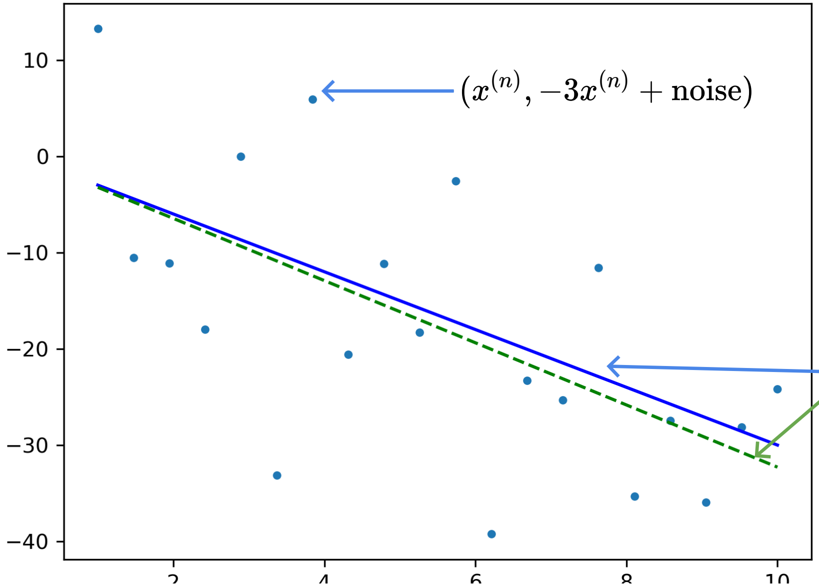
```
def gradient(X, y, w):
    N,D = X.shape
    yh = np.dot(X, w)
    grad = np.dot(X.T, yh - y) / N
    return grad
```

Example: GD for Linear Regression

applying this to to fit toy data ←

```
#D = 1
N = 20
X = np.linspace(1,10, N)[:,None]
y_truth = np.dot(x, np.array([-3.]))
y = y_truth + 10*np.random.randn(N)
```

single feature (intercept is zero)



using direct solution method

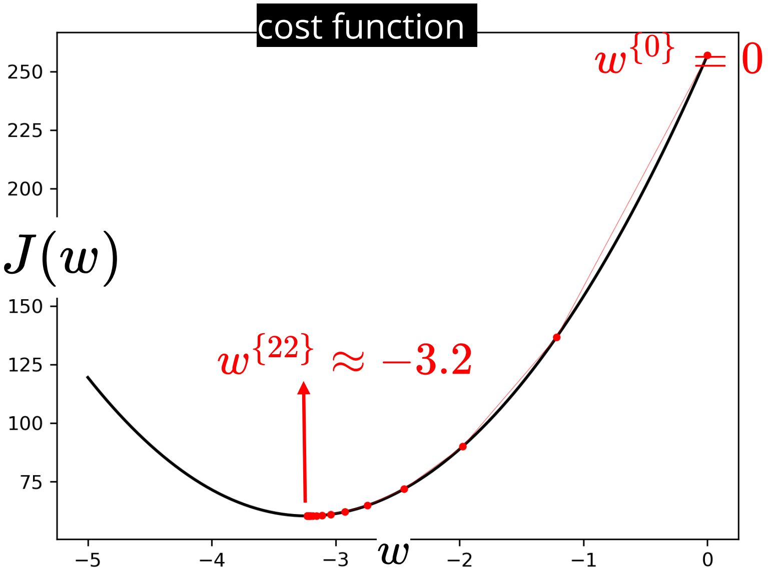
$$w = (X^T X)^{-1} X^T y \approx -3.2$$

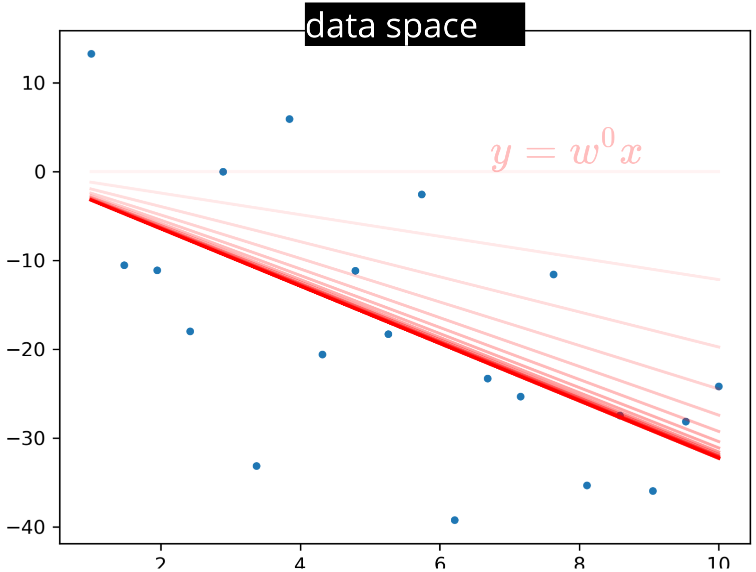
$$y = wx$$

$$y = -3x$$

Example: GD for Linear Regression

After 22 iterations of Gradient Descent $w^{\{t+1\}} \leftarrow w^{\{t\}} - .01 \nabla J(w^{\{t\}})$



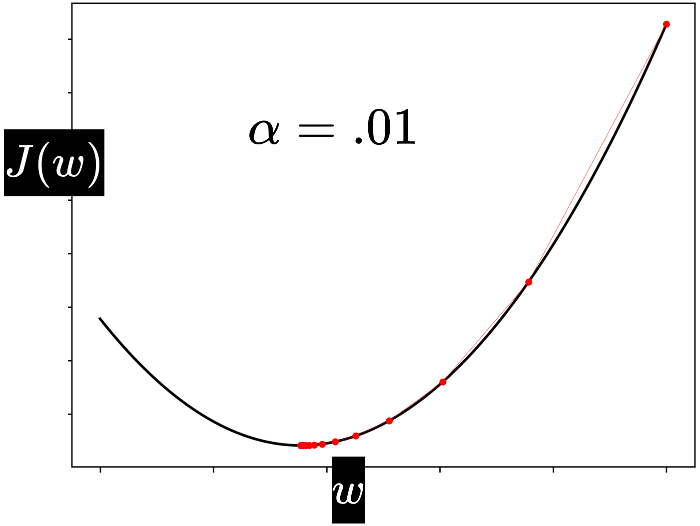


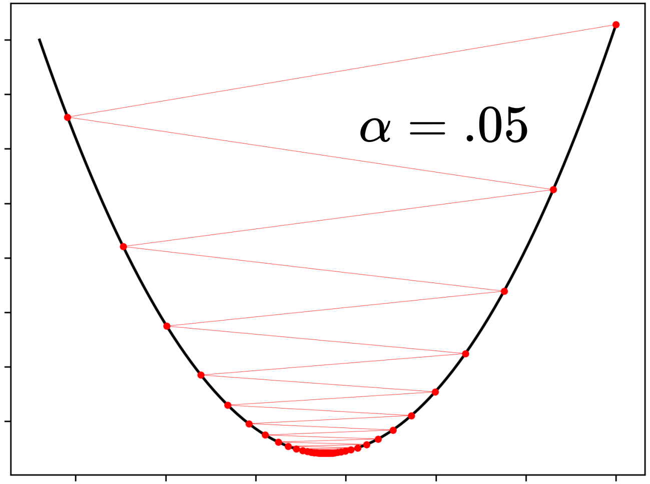
Learning rate α

Learning rate has a significant effect on GD

too small: may take a long time to converge

too large: it overshoots



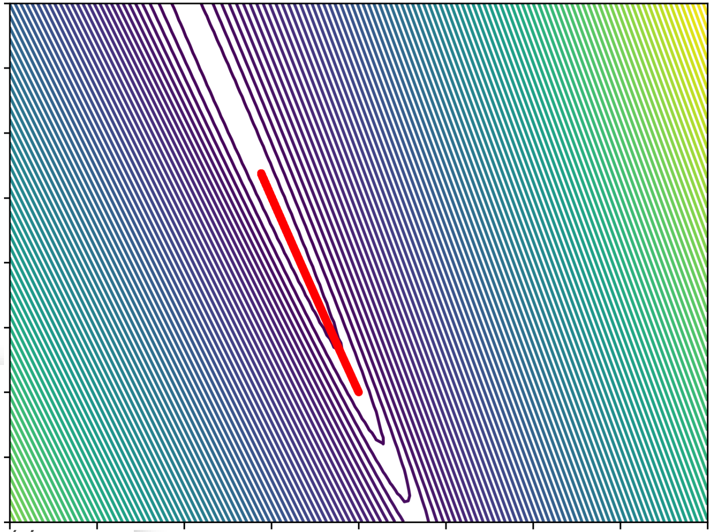


GD for logistic Regression

example: *logistic regression for Iris dataset* (D=2, lr=.01)

```
def GradientDescent(X, # N x D
                    y, # N
                    lr=.01, # learning rate
                    eps=1e-2, # termination codition
                   ):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    while np.linalg.norm(g) > eps:
        g = gradient(X, y, w)
        w = w - lr*g
    return w
```

```
def gradient(X, y, w):
    yh = logistic(np.dot(X,
    grad = np.dot(X.T, yh -
    return grad
```



Stochastic Gradient Descent

we can write the cost function as a 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 $\nabla J(w) = \mathbb{E}[\nabla J_n(w)]$

Stochastic Gradient Descent

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

contour plot of the cost function + batch gradient update $w \leftarrow w - \alpha \nabla J(w)$

with small learning rate: guaranteed improvement at each step

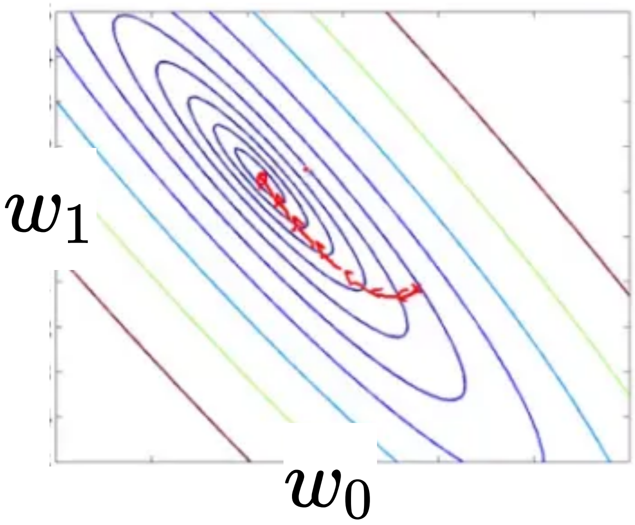


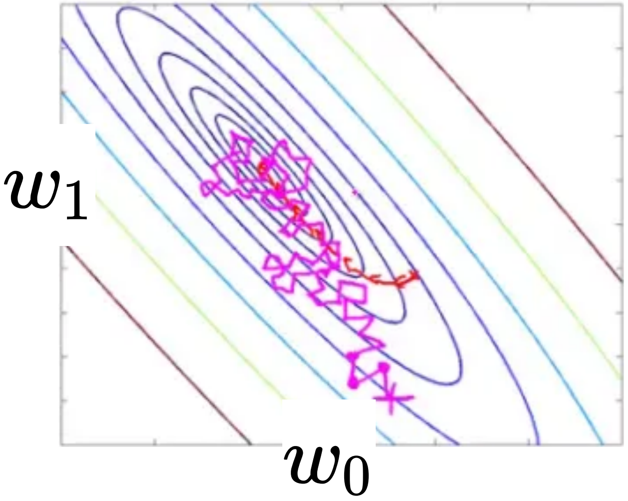
image:https://jaykanidan.wordpress.com

Stochastic Gradient Descent

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

using stochastic gradient $w \leftarrow w - \alpha \nabla J_n(w)$

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 $\mathcal{O}(D)$

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

image:https://jaykanidan.wordpress.com

Example: SGD for logistic regression

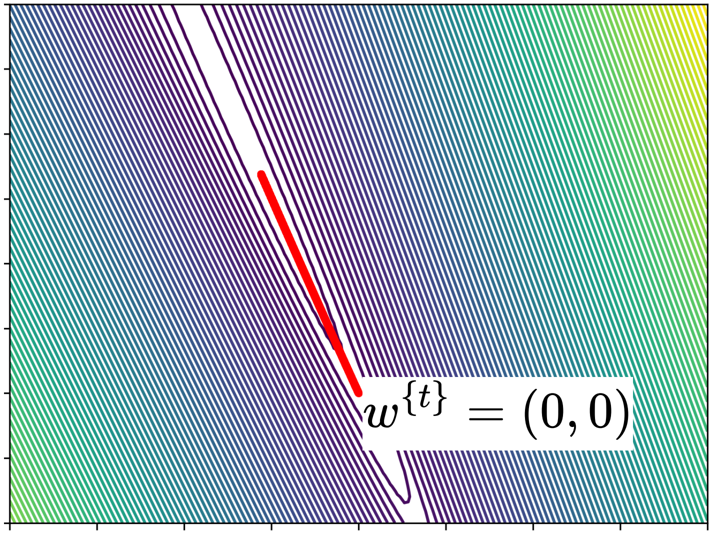
setting 1: using batch gradient

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

```
def GradientDescent(X, # N x D
                    y, # N
                    lr=.01, # learning rate
                    eps=1e-2, # termination codition
                   ):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    while np.linalg.norm(g) > eps:
        g = gradient(X, y, w)
        w = w - lr*g
    return w
```

```
def gradient(X, y, w):
    N, D = X.shape
    yh = logistic(np.dot(X, w))
    grad = np.dot(X.T, yh - y) / N
    return grad
```

after 8000 iterations

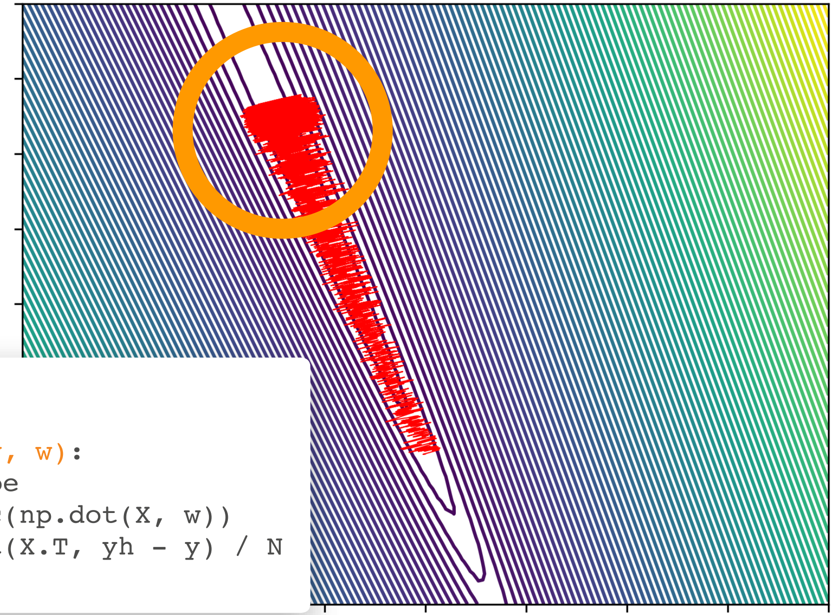


Example: SGD for logistic regression

setting 2: using stochastic gradient

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

```
def StochasticGradientDescent(
                                        X, # N x D
                         y, # N
                         lr=.01, # learning rate
                         eps=1e-2, # termination codition
                        ):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    while np.linalg.norm(g) > eps:
        n = np.random.randint(N)
        g = gradient(X[[n],:], y[[n]], w)
        w = w - lr*g
    return w
```



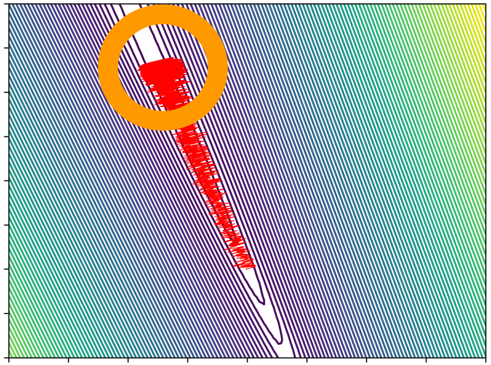
```
def gradient(X, y, w):
    N, D = X.shape
    yh = logistic(np.dot(X, w))
    grad = np.dot(X.T, yh - y) / N
    return grad
```

Convergence of SGD

stochastic gradients are not zero at optimum

how to guarantee convergence?

schedule to have a smaller learning rate over time



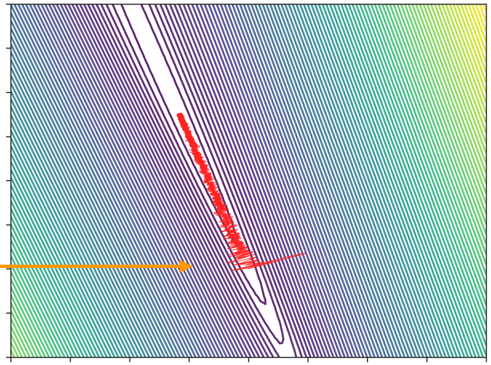
Robbins Monro

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

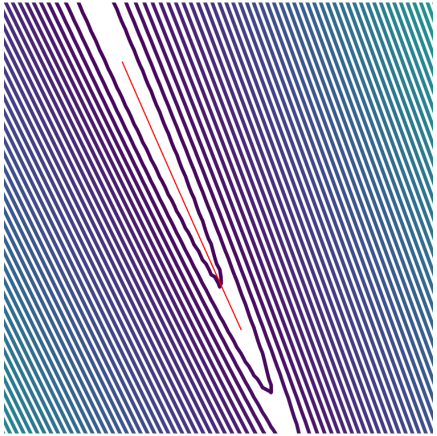
use a minibatch to produce gradient estimates

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

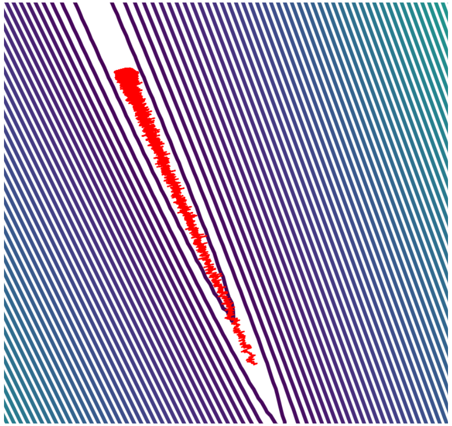
$\mathbb{B} \subseteq \{1, \ldots, N\}$ a subset of the dataset

```python
def MinibatchSGD(X, y, lr=.01, eps=1e-2, bsize=8):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    while np.linalg.norm(g) > eps:
        minibatch = np.random.randint(N, size=(bsize))
        g = gradient(X[minibatch,:], y[inibatch], w)
        w = w - lr*g
    return w
```

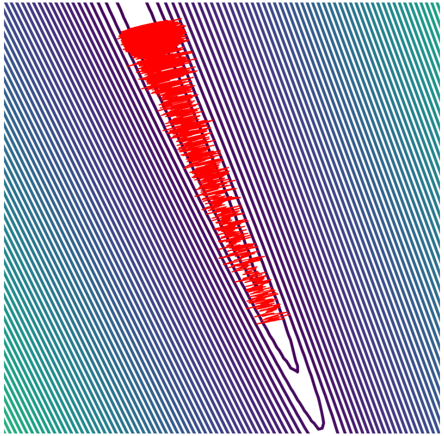
GD full batch



SGD minibatch-size=16



SGD minibatch-size=1



Momentum

to help with oscillations of SGD (or even full-batch GD):

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

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

$$w^{\{t\}} \leftarrow w^{\{t-1\}} - \alpha \Delta w^{\{t\}}$$

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

to help with oscillations of SGD (or even full-batch GD):

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

```
def MinibatchSGD(X, y, lr=.01, eps=1e-2, bsize=8, beta=.99):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    dw = 0
    while np.linalg.norm(g) > eps:
        minibatch = np.random.randint(N, size=(bsize))
        g = gradient(X[minibatch,:], y[inibatch], w)
        dw = (1-beta)*g + beta*dw
        w = w - lr*dw
    return w

```

Momentum

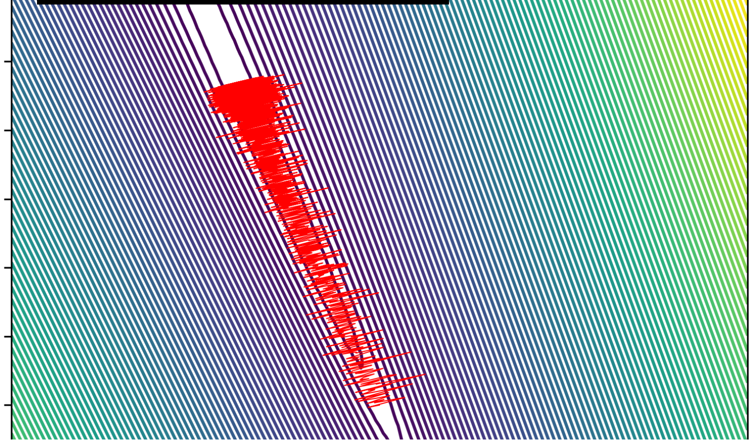
Example: logistic regression

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

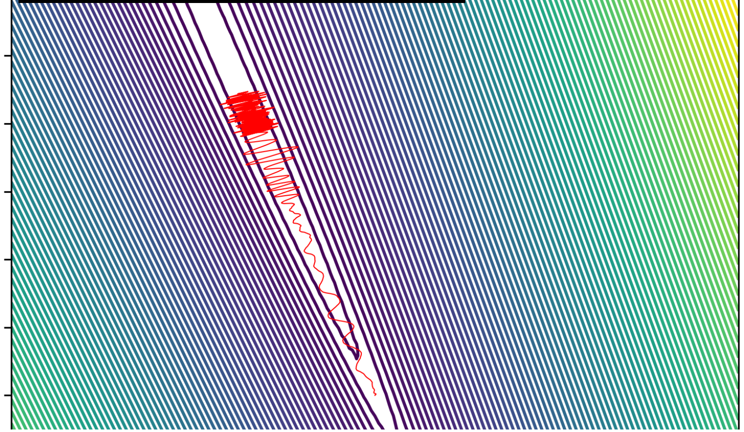
$$w^t \leftarrow w^{t-1} - \alpha \Delta w^t$$

no momentum

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



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



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)

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

the learning rate is adapted to previous updates

ϵ is to avoid numerical issues

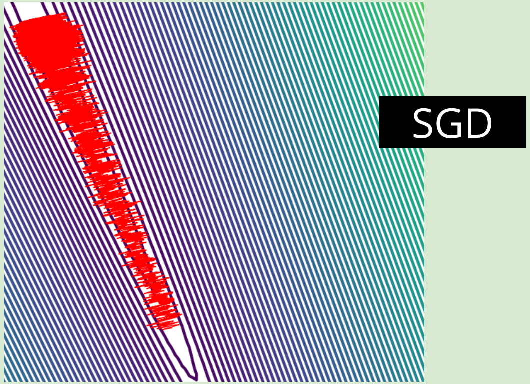
useful when parameters are updated at different rates (*e.g., NLP*)

Adagrad (Adaptive gradient)

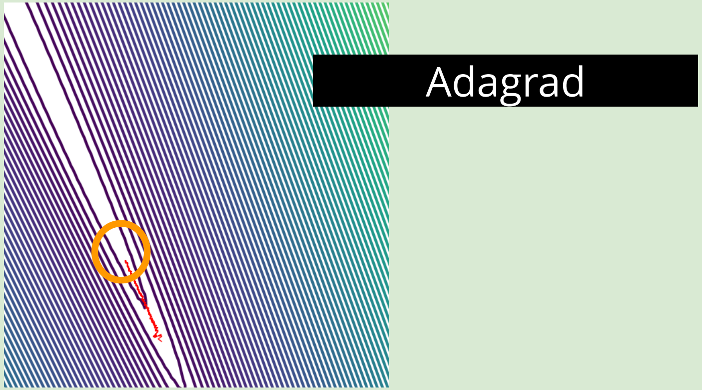
different learning rate for each parameter w_d

make the learning rate adaptive

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



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



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)

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

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

identical to Adagrad

```
def RMSprop(X, y, lr=.01, eps=1e-2, bsize=8, gamma=.9, epsilon=1e-8):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    S = 0
    while np.linalg.norm(g) > eps:
        minibatch = np.random.randint(N, size=(bsize))
        g = gradient(X[minibatch,:], y[inibatch], w)
        S = (1-gamma)*g**2 + gamma*S
        w = w - lr*g/np.sqrt(S + epsilon)
    return w
```

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**:

$$M^{\{t\}} \leftarrow \beta_1 M^{\{t-1\}} + (1-\beta_1)\nabla J(w^{\{t-1\}})$$

identical to method of momentum
(moving average of the first moment)

$$S^{\{t\}} \leftarrow \beta_2 S^{\{t-1\}} + (1-\beta_2)\nabla J(w^{\{t-1\}})^2$$

identical to RMSProp
(moving average of the second moment)

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

Adam (Adaptive Moment Estimation)

Adam combines thee two:

$$M^{\{t\}} \leftarrow \beta_1 M^{\{t-1\}} + (1-\beta_1)\nabla J(w^{\{t-1\}})$$

identical to method of momentum
(moving average of the first moment)

$$S^{\{t\}} \leftarrow \beta_2 S^{\{t-1\}} + (1-\beta_2)\nabla J(w^{\{t-1\}})^2$$

identical to RMSProp
(moving average of the second moment)

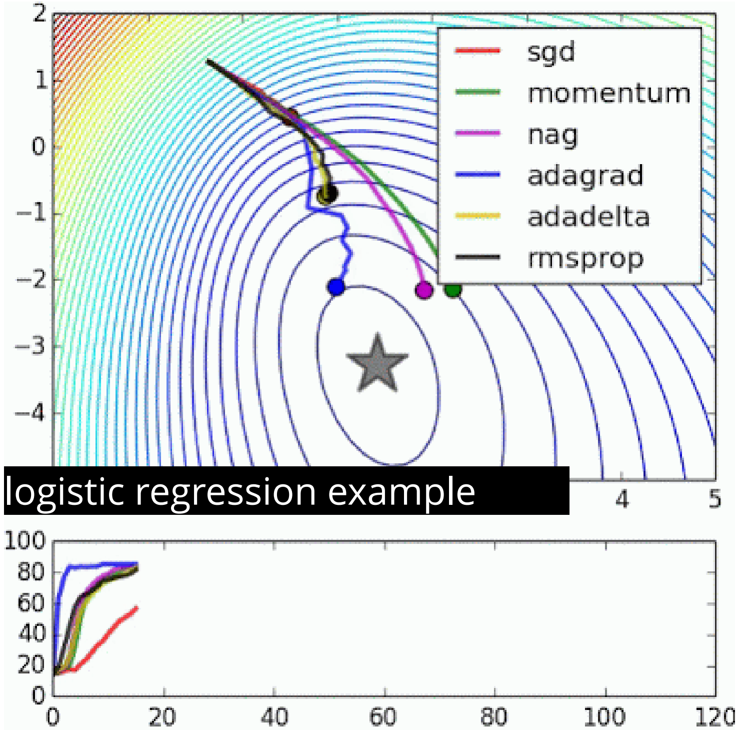
$$w^{\{t\}} \leftarrow w_d^{\{t-1\}} - \frac{\alpha \hat{M}^{\{t\}}}{\sqrt{\hat{S}^{\{t\}}+\epsilon}} \nabla J(w^{\{t-1\}})$$

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

$$\hat{M}^{\{t\}} \leftarrow \frac{M^{\{t\}}}{1-\beta_1^t} \qquad \hat{S}^{\{t\}} \leftarrow \frac{S^{\{t\}}}{1-\beta_2^t}$$

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

In practice



logistic regression example

image:Alec Radford

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

Adding L_2 regularization

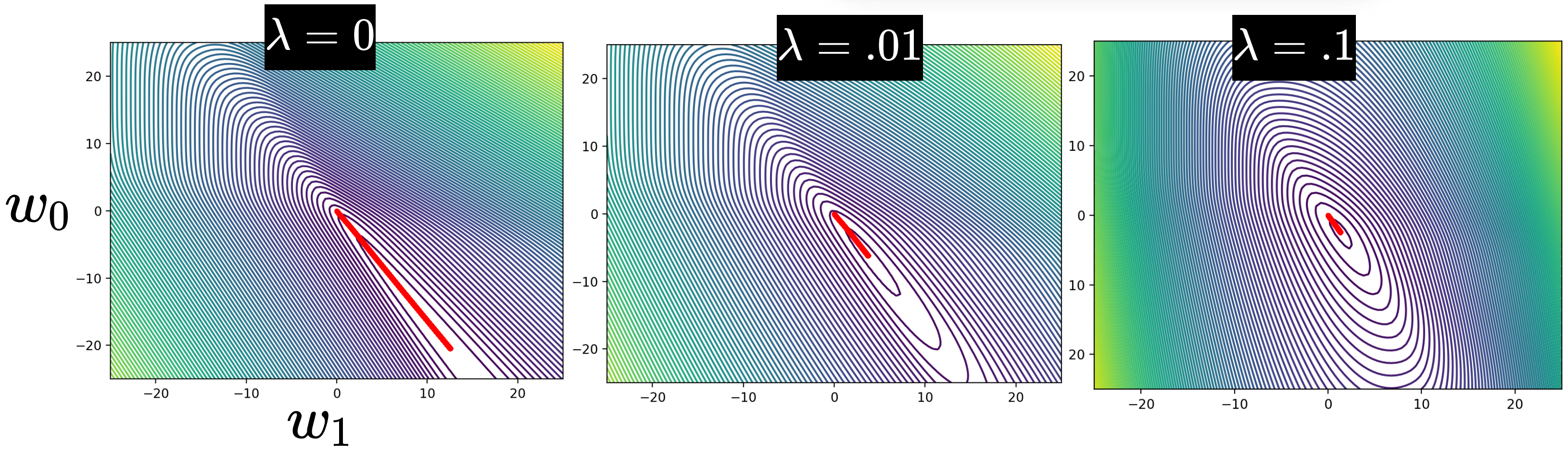
do not penalize the bias w_0

L2 penalty makes the optimization easier too!

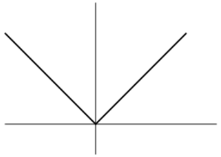
note that the optimal w_1 shrinks

```
def gradient(X, y, w, lambdaa):
    N,D = X.shape
    yh = logistic(np.dot(X, w))
    grad = np.dot(X.T, yh - y) / N
    grad[1:] += lambdaa * w[1:]
    return grad
```

weight decay



Subgderivatives



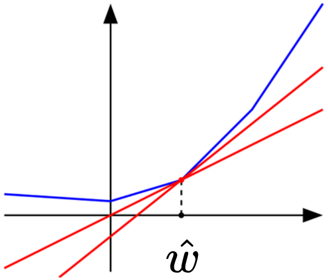
L1 penalty is no longer smooth or differentiable (at 0)

extend the notion of derivative to non-smooth functions

sub-differential is the set of all **sub-derivatives** at a point

$$\partial f(\hat{w}) = \left[\lim_{w \to \hat{w}^-} \frac{f(w)-f(\hat{w})}{w-\hat{w}}, \lim_{w \to \hat{w}^+} \frac{f(w)-f(\hat{w})}{w-\hat{w}}\right]$$

if $\boldsymbol{f}$ is differentiable at $\hat{w}$ then sub-differential has one member $\frac{d}{dw} f(\hat{w})$

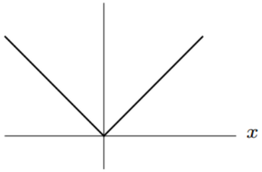


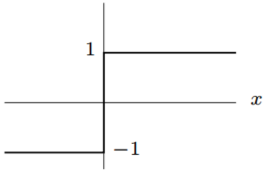
another expression for sub-differential

$$\partial f(\hat{w}) = \{g \in \mathbb{R} |\ f(w) > f(\hat{w}) + g(w - \hat{w})\}$$

Subgradient

example subdifferential absolute $f(w) = |w|$





$$\partial f(0) = [-1, 1]$$

$$\partial f(w \neq 0) = \{\mathrm{sign}(w)\}$$

recall, **gradient** was the vector of **partial derivatives**

subgradient is a vector of **sub-derivatives**

subdifferential for functions of multiple variables

$$\partial f(\hat{w}) = \{g \in \mathbb{R}^D | f(w) > f(\hat{w}) + g^T(w - \hat{w})\}$$

we can use sub-gradient with diminishing step-size for optimization

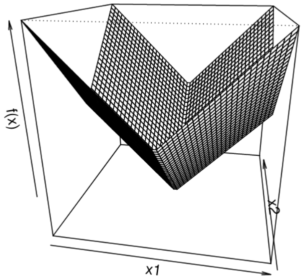


image credit: G. Gordon

Adding L_1 regularization

L1-regularized *linear regression* has efficient solvers

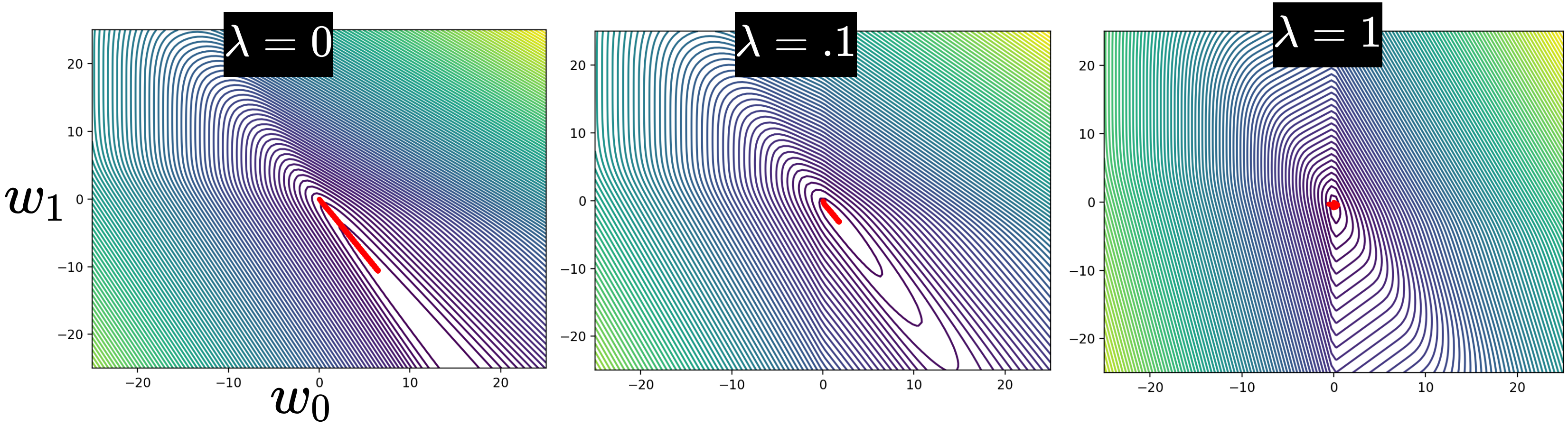
subgradient method for L1-regularized logistic regression

do not penalize the bias w_0

using **diminishing learning rate**

note that the optimal w_1 **becomes 0**

```
def gradient(X, y, w, lambdaa):
    N,D = X.shape
    yh = logistic(np.dot(X, w))
    grad = np.dot(X.T, yh - y) / N
    grad[1:] += lambdaa * np.sign(w[1:])
    return grad
```



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

Adding regularization can also help with optimization

Adadelta

solve the problem of diminishing step-size with Adagrad

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

also gets rid of a "learning rate" altogether

- use another moving average for that!

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

moving average of the sq. gradient

$$U^{\{t\}} \leftarrow \gamma U^{\{t-1\}} + (1-\gamma)\Delta w^{\{t-1\}}$$

moving average of the sq. updates

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

square root of the ratio of the above is used as the adaptive learning rate

$$w^{\{t\}} \leftarrow w^{\{t-1\}} + \Delta w^{\{t\}}$$