Machine Learning & Pattern Recognition

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Iterative Optimization Technique

Optimization Methods

- Optimization: either minimize or maximize some function $f(x)$ by altering x.
- In most cases, optimizitaion refers to the minimization of $f(x)$.

Maximization $f(x)$ ⟺ **Minimization** $-f(x)$

- $f(x)$: objective function, cost function, loss function, error function.
- The value that minimize $f(x)$: $x^* = \arg\min f(x)$.

Optimization Methods

- **Deterministic Optimization**
  - The data for the given problem are known accurately.
- **Stochastic Optimization**
  - Refers to a collection of methods for minimizing or maximizing an objective function when randomness is present.

Deterministic Optimization

- First-order methods: methods that use only the gradient.
- Second-order methods: methods that also use the Hessian matrix.

$$\boldsymbol{H}(f)_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(\boldsymbol{x})$$

$\boldsymbol{x}$: multiple input dimensions.

Gradient Descent [Cauchy 1847]

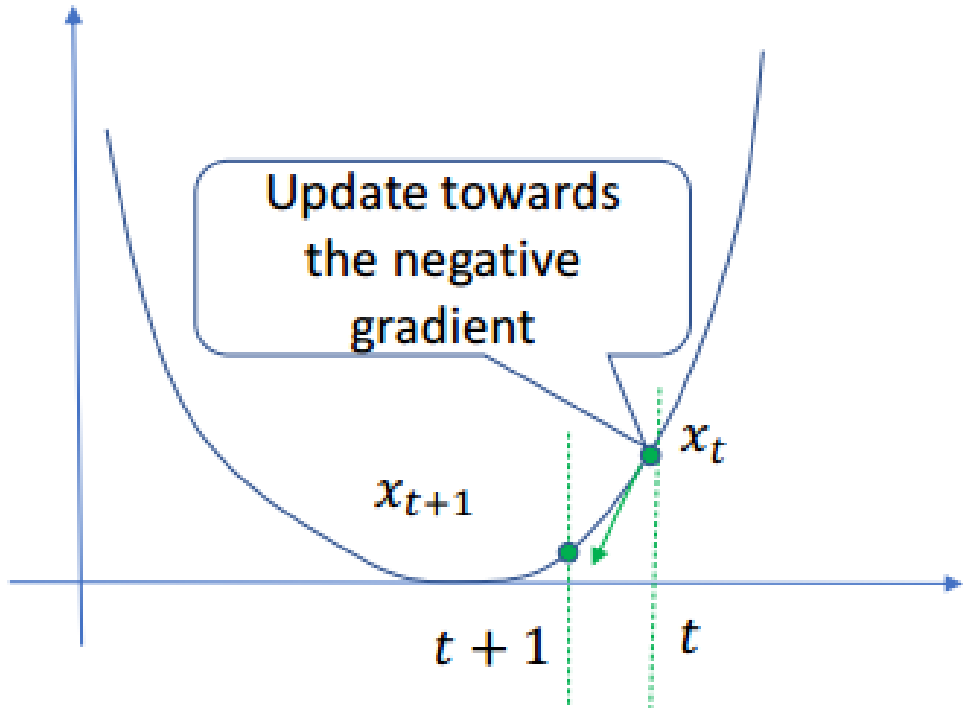
- Motivation: to minimize the local first-order Taylor approximation of f

$$\min_x f(x) \approx \min_x f(x_t) + \nabla f(x_t)^T (x - x_t)$$

- Update rule:

$$x_{t+1} = x_t - \eta_t \nabla f(x_t)$$

Where $\eta_t > 0$ is the step-size (learning rate).



Interpretation1

- At each iteration, consider the expansion

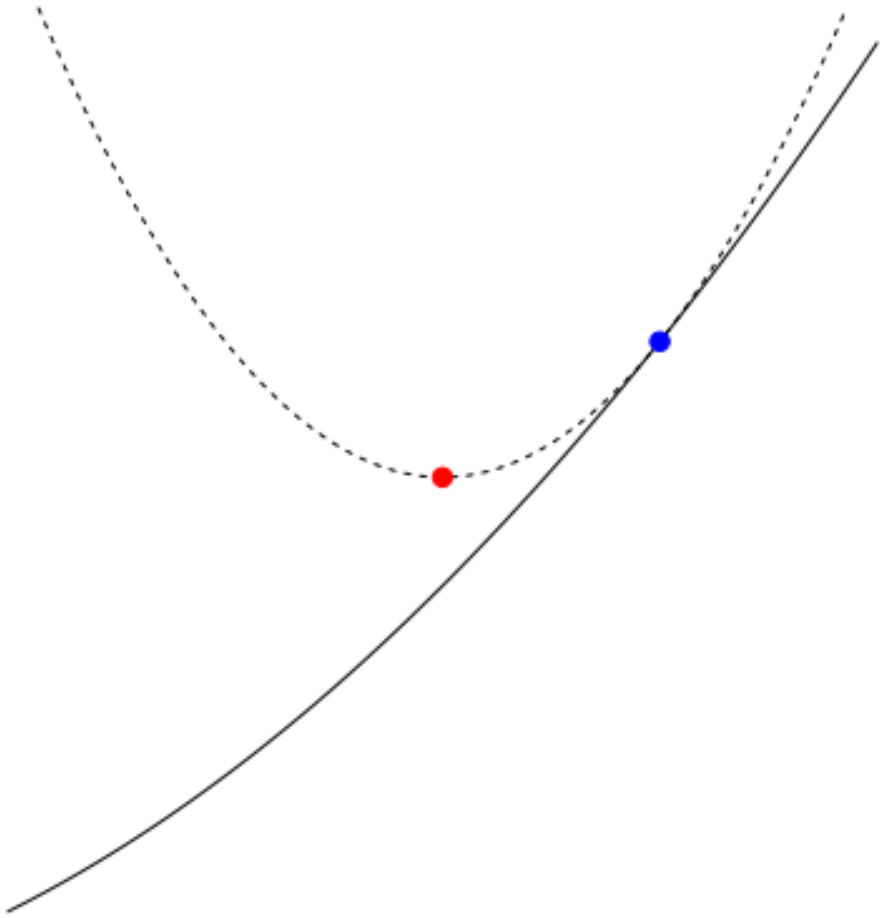
$$f(y) \approx f(x_t) + \nabla f(x_t)^T (y - x_t) + \frac{1}{2\eta_t} \|y - x_t\|^2$$

Linear approximation of f Proximity term with weight $\frac{1}{2\eta_t}$

- Quadratic approximation, replacing usual $\nabla^2 f(x)$ by $\frac{1}{\eta_t} I$:

$$x_{t+1} = x_t - \eta_t \nabla f(x_t)$$

Interpretation1



Blue point is x_t, red point is x_{t+1}.

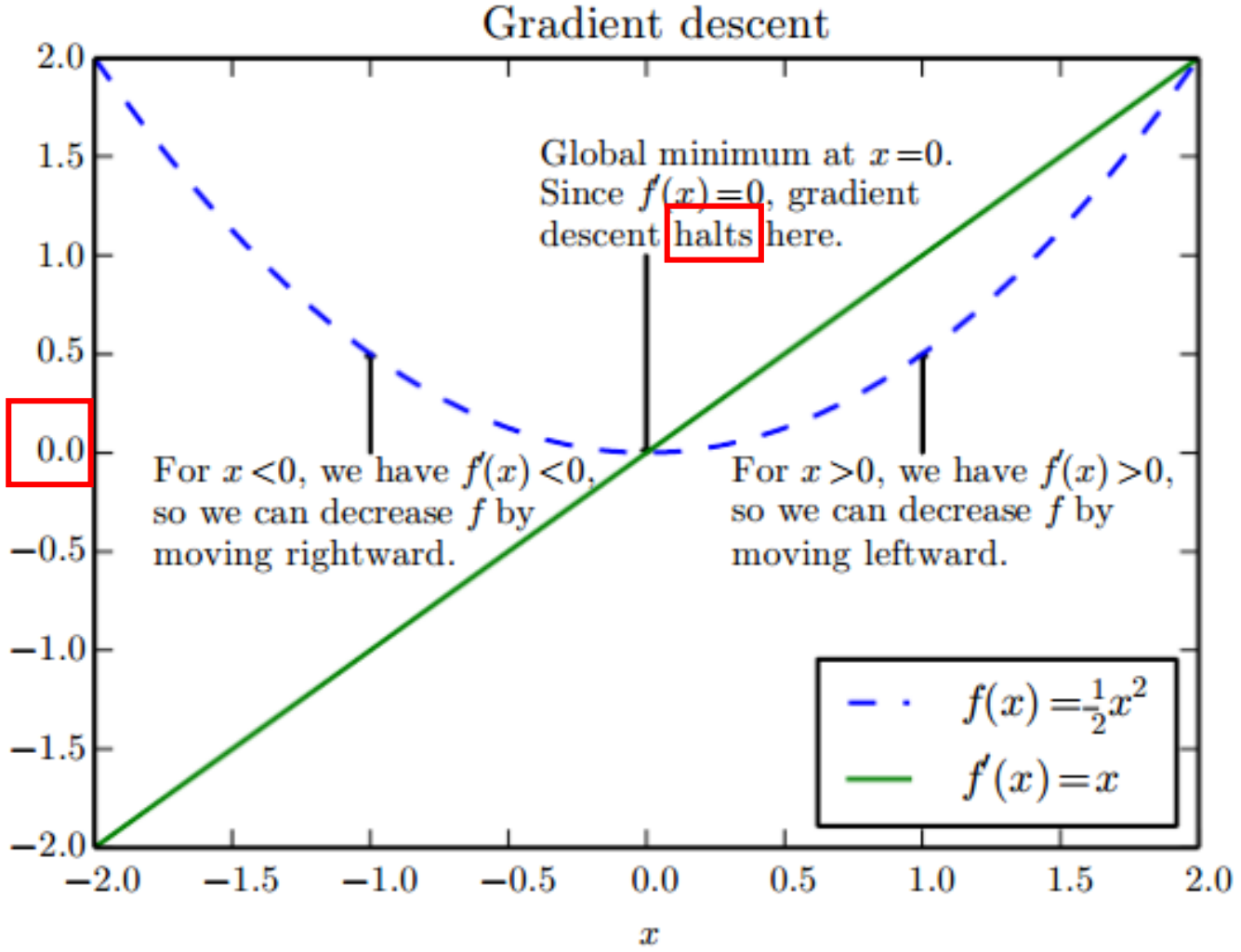
Interpretation2

- Reduce $f(x)$ by moving x in small steps with opposite sign of the derivative.

- Update rule:

$$x_{t+1} = x_t - \eta_t \nabla f(x_t)$$

- Critical/stationary points: Points where $f'(x) = 0$ 驻点

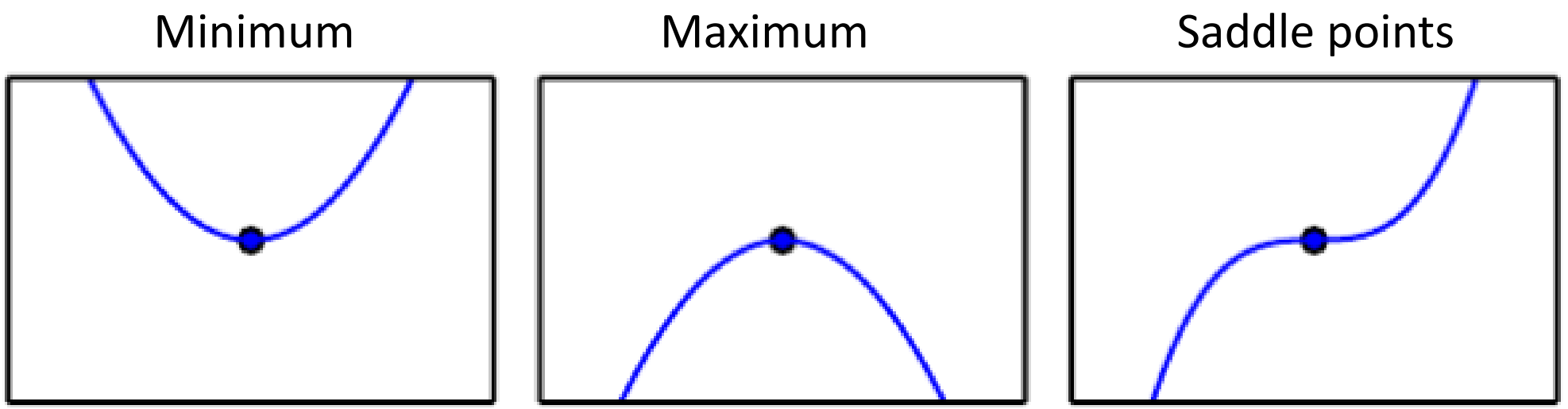


An illustration of gradient descent.

Global VS Local Minimum

- Global minimum: a point that obtains the absolute lowest value of $f(x)$.
- Local minimum: a point where $f(x)$ is higher than at all neighboring points.
- Saddle points: some critical points are neither maxima or minima. 鞍点

Types of critical points



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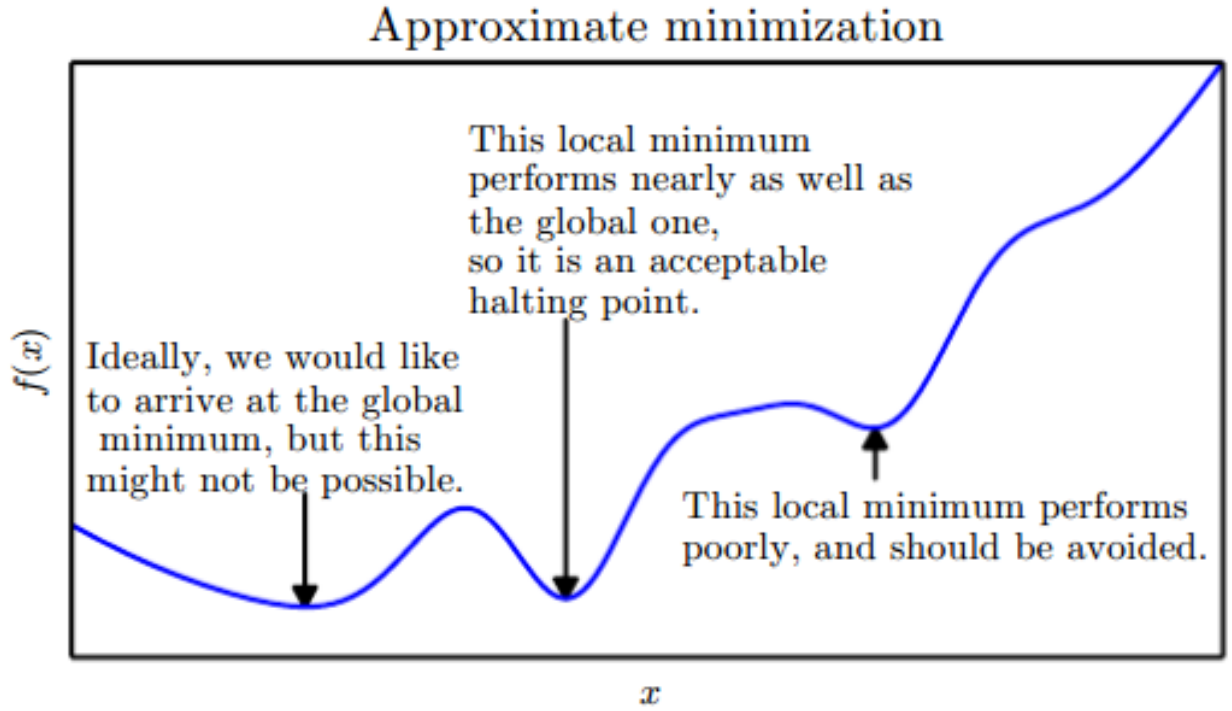
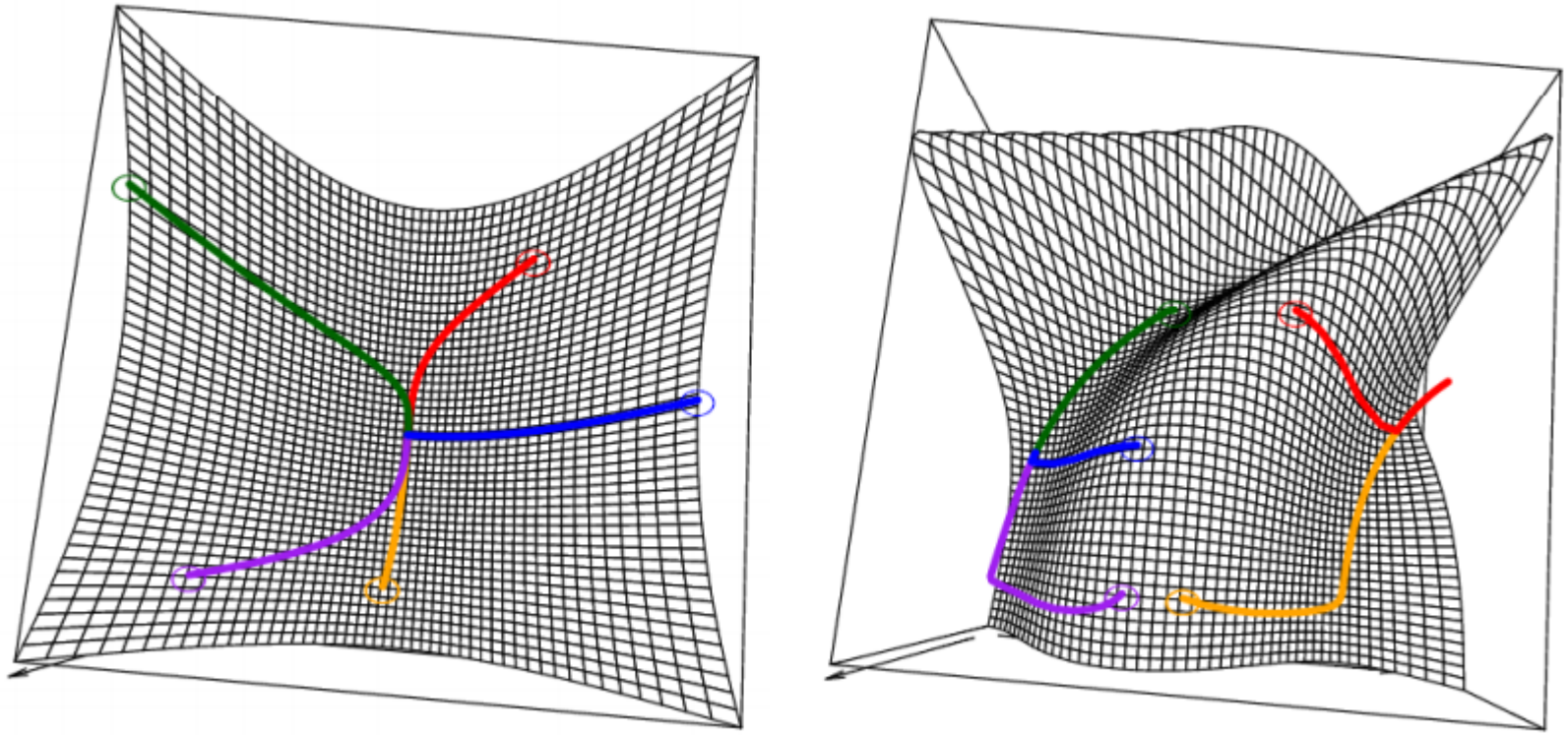


Different Starting Points

- Gradient Descent with different starting points are illustrated in different colors.



(a) Convex function

(b) Non-convex function

- (a): Strictly convex function: Converge to the global optimum.
- (b): Non-convex function: Different paths may end up at different local optima.

Gradient Descent [Cauchy 1847]

$$x_{t+1} = x_t - \eta_t \nabla f(x_t)$$

How to choose step sizes?

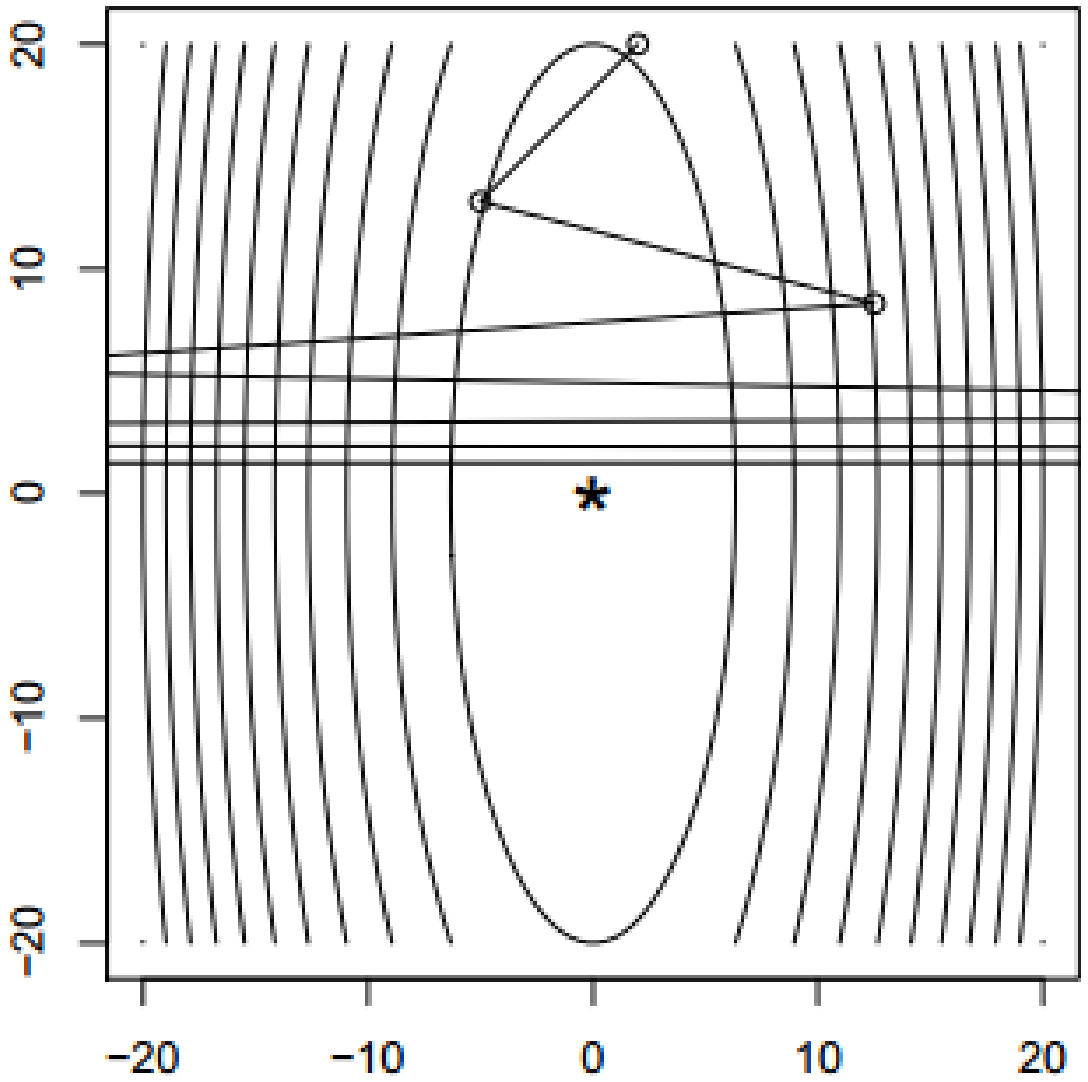
- Gradient Descent requires a step size η controlling the amount of gradient updated to the current point at each iteration.
- It is naïve to set $\eta_t = \eta$ for all iterations.

Fixed Step Sizes

Considering $f(x) = (10x_1^2 + x_2^2)/2$

If η is too big, can lead to divergence.

- The learning function oscillates away from the optimal point.
- As shown, it oscillates after 8 steps.

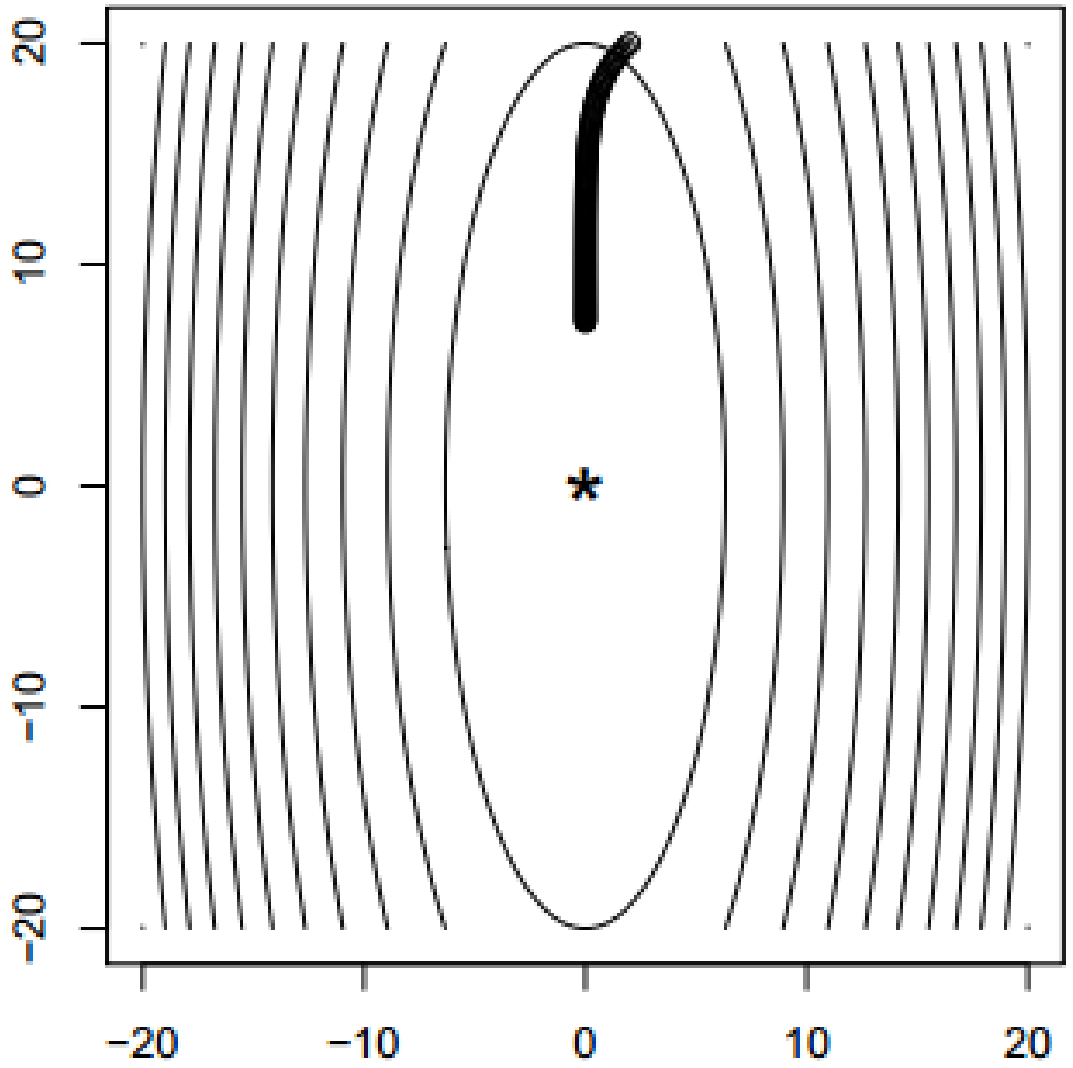


Fixed Step Sizes

Considering $f(x) = (10x_1^2 + x_2^2)/2$

If η is too small, takes longer time for the function to converge.

- As shown, GD after 100 steps.

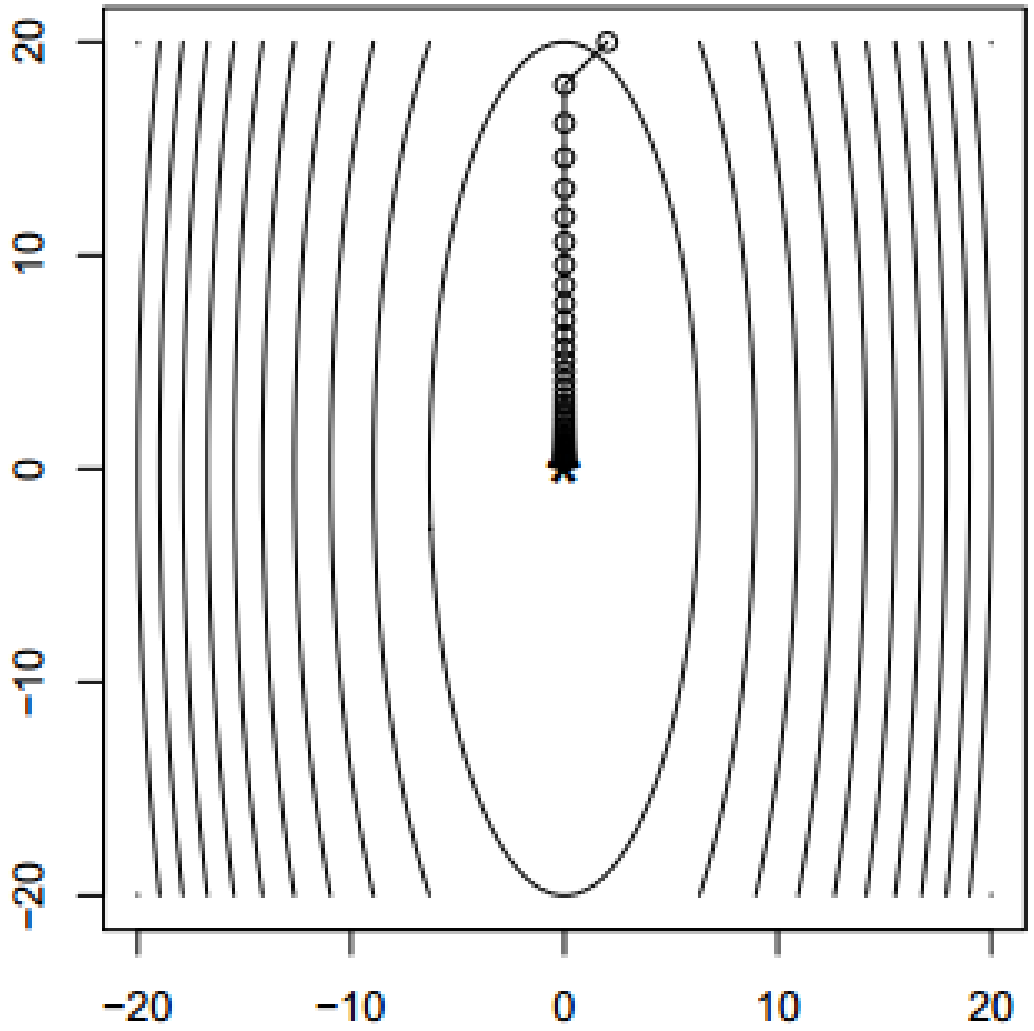


Fixed Step Sizes

Considering $f(x) = (10x_1^2 + x_2^2)/2$

Same example, gradient descent after 40 appropriately sized steps.

This porridge is too hot! - too cold! -juuussst right!



Line Search

- For algorithm 1, we need to find a search direction d_k
  - $f(x_k + \alpha d_k) < f(x_k)\ \forall \alpha \in [0, \epsilon] \ \leftrightarrow\ \nabla f(x_k)^T d_k < 0$

Algorithm 1: General gradient method with line search

1 Specify x_0 as an initial guess for the minimum and $k = 0$;
2 **repeat**
3 | Compute a search direction d_k;
4 | Choose a step size $\alpha_k > 0$ to minimize $h(\alpha) = f(x_k + \alpha d_k)$;
5 | Update $x_{k+1} = x_k + \alpha_k d_k$ and $k = k + 1$;
6 **until** *Convergence* ;

Exact Line Search

- Given the search direction d_k, the line search need to solve,
  - $\alpha = \arg\min_{\alpha \geq 0} h(\alpha) = \arg\min_{\alpha \geq 0} f(x_k + \alpha d_k)$
- If $h(\alpha)$ is differentiable and convex, then the optimal should satisfy,

$$h'(\alpha) = \nabla f(x_k + \alpha d_k)^T d_k = 0$$

- Since $\nabla f(x_k)^T d_k < 0$, i.e., $h'(0) < 0$.
- If we can find $\hat{\alpha}$ such that $h'(\hat{\alpha}) > 0$, then there must exist $\alpha^* \in [0, \hat{\alpha})$ such that $h'(\alpha^*) = 0$.
- There are many iterative algorithms to find the estimate of α^*.

Bisection Line Search

In this method, we begin with an interval $[\alpha_l, \alpha_h]$ $(h'(\alpha_l) < 0, h'(\alpha_h) > 0)$ and divide the interval in two halves, i.e., $[\alpha_l, (\alpha_l + \alpha_h)/2]$ and $[(\alpha_l + \alpha_h)/2, \alpha_h]$.

A next search interval is chosen according to the sign of $h'((\alpha_l + \alpha_h)/2)$.

Algorithm 2: Bisection Line Search algorithm

```
1  Initialize α_l = 0, α_h = α̂ and k = 0// h'(α_h) > 0;
2  while k < MAX do // prevent infinite loop
3      Set α_m = (α_l + α_h)/2;
4      if h'(α_m) ≈ 0 or α_h − α_l < ϵ then // solution found!
5          return α_m;
6      else if h'(α_m) > 0 then
7          update α_h = α_m;
8      else
9          update α_l = α_m;
10     k = k + 1;
```

Bisection Line Search

- Bisection is accurate but may be expensive in practice.
- Usually not possible to do this minimization exactly.
- Need cheap method guaranteeing sufficient accuracy.
- Inexact line search method, much more efficient.

Backtracking Line Search—Armijo Rule

- A line search method to determine the maximum amount (step size) to move along a given search direction d_k.
  - Starts with a large estimate of the step size α for movement;
  - Iteratively shrinking the step size (i.e., "backtracking") until a sufficient decrease of the $f(x_k) - f(x_k + \alpha d_k)$.

$$f(x_k + \alpha d_k) \leq f(x_k) + c_1 \alpha f'(x_k)^T d_k$$

$f: \mathbb{R}^n \to \mathbb{R}, c_1 \in (0,1), \alpha$: step size, d_k is the search direction which satisfies $\nabla f(x_k)^T d_k < 0$.

Backtracking Line Search—Armijo Rule

$h'(\alpha) = \nabla f(x_k + \alpha d_k)^T d_k$

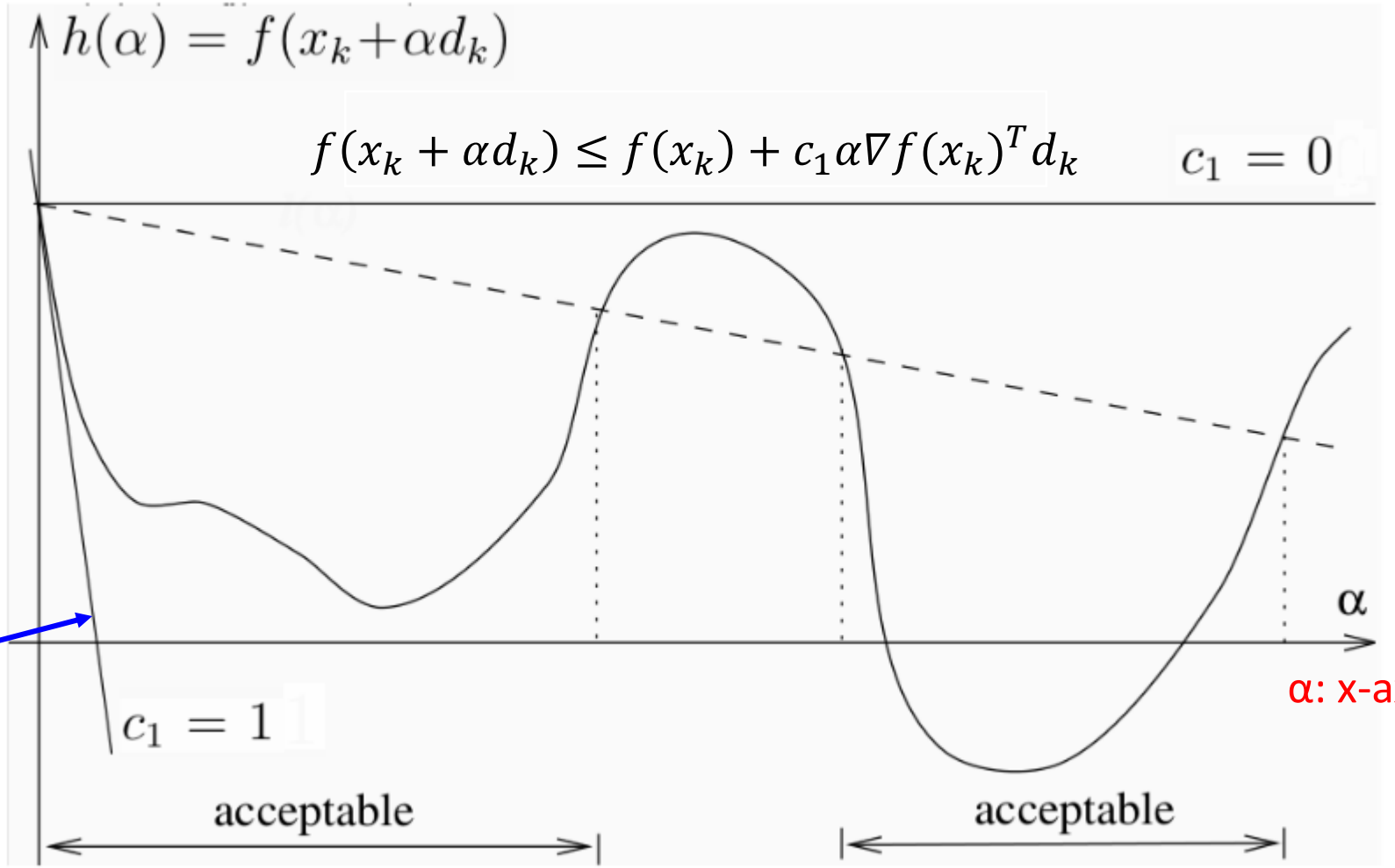
Slope at $\alpha = 0$

$h'(0) = \nabla f(x_k)^T d_k$

$h(0) = f(x_k)$

The function of the tangent,

$l(\alpha) = f(x_k) + \alpha \nabla f(x_k)^T d_k$



α: x-axis.

Armijo condition for backtracking line search

Backtracking Line Search—Armijo Rule

- As long as α is sufficient small, α must satisfy the Armijo rule.
- That is why we need to start with a large step and then shrink it.

Algorithm 3: Backtracking Line Search with Armijo condition

Input: $c_1 \in (0,1)$,$\tau \in (0,1)$,search direction d and step size α_0

Initialize $k = 0$;

while $f(x + \alpha_k d) > f(x) + c_1 \alpha_k f'(x)^T d$ **do**

    update $\alpha_{k+1} = \tau \alpha_k$;

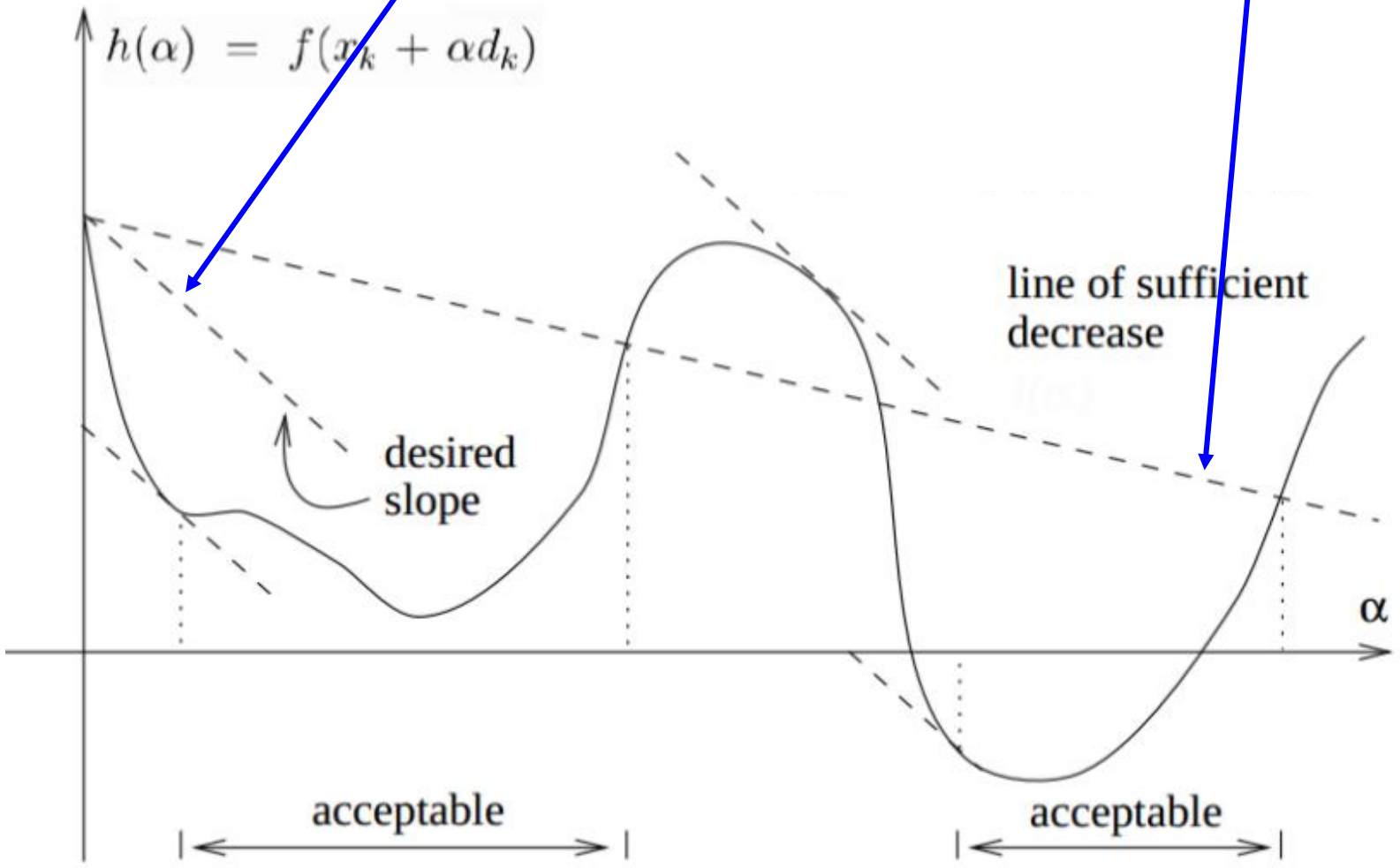
    $k = k + 1$;

return α_k;

Backtracking Line Search—Wolfe Rule

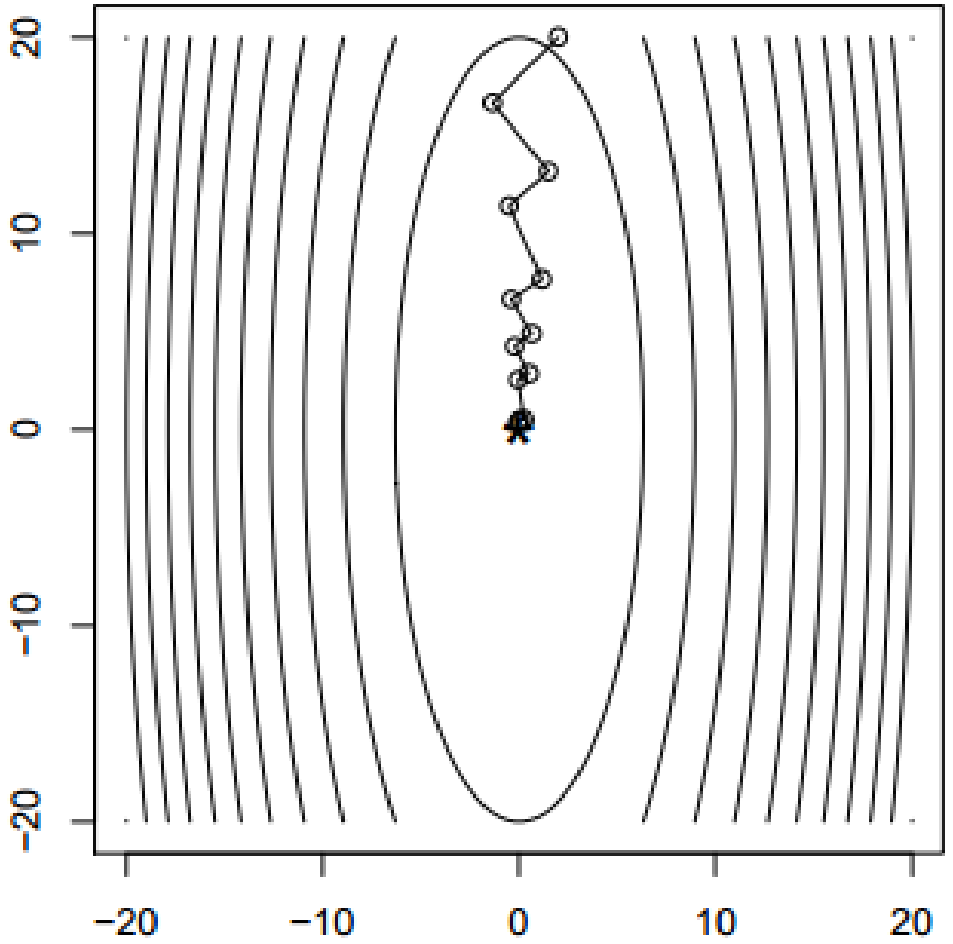
Armijo Rule: $f(x_k + \alpha d_k) \leq f(x_k) + c_1 \alpha \nabla f(x_k)^T d_k$

Curvature Condition: $f'(x_k + \alpha d_k)^T d_k \geq c_2 f'(x_k)^T d_k$



Backtracking Line Search

- Backtracking picks up roughly the right step size (13 steps):
- Here $\beta = 0.8$. (Recommend $\beta \in (0.1, 0.8)$)



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Newton's Methods

- Motivation: to minimize the local second-order Taylor approximation of f.

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \approx \min_{\boldsymbol{x}} f(\boldsymbol{x}_t) + \nabla f(\boldsymbol{x}_t)^T(\boldsymbol{x} - \boldsymbol{x}_t) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_t)^T \nabla^2 f(\boldsymbol{x}_t)(\boldsymbol{x} - \boldsymbol{x}_t)$$

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- Take the derivative of $\boldsymbol{x}$ on both side, we have,

$$\frac{df(\boldsymbol{x})}{d\boldsymbol{x}} = \nabla f(x_t) + \nabla^2 f(\boldsymbol{x}_t)(\boldsymbol{x} - \boldsymbol{x}_t) = \mathbf{0}$$

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- Update rule: suppose $\nabla^2 f(x_t)$ is positive definite,

$$\boldsymbol{x} = \boldsymbol{x}_t - [\nabla^2 f(x_t)]^{-1} \nabla f(x_t)$$

Newton's Methods

- Motivation: to minimize the local second-order Taylor approximation of f.

$$\min_x f(x) \approx \min_x f(x_t) + f'(x_t)(x - x_t) + \frac{1}{2} f''(x_t)(x - x_t)^2$$

- Take the derivative of x on both side, we have,

$$f'(x) = f'(x_t) + f''(x_t)(x - x_t) = 0$$

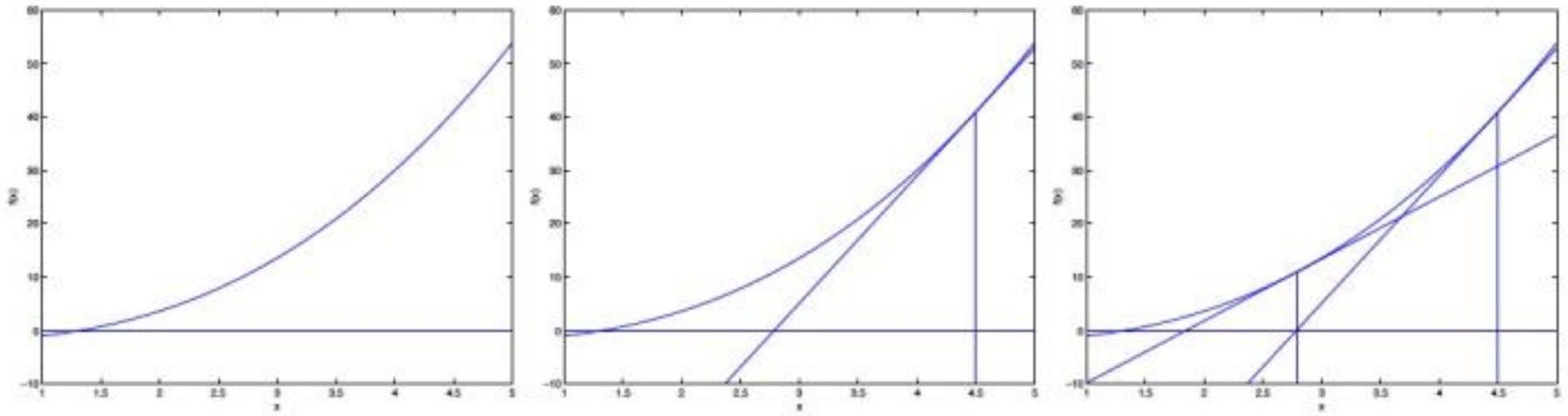
- Update rule: suppose $f''(x_t) \neq 0$,

$$x = x_t - \frac{f'(x_t)}{f''(x_t)}$$

Newton's Methods

- In numerical analysis, Newton's Methods is to find successively better approximations to the roots of a real-valued function, $(\text{i.e, } z\text{: } f(z) = 0)$.

$$z = z_t - \frac{f(z_t)}{f'(z_t)}$$



- In optimization, we want to find the stationary point $f'(x_t) = 0$, i.e.,

$$x = x_t - \frac{f'(x_t)}{f''(x_t)}$$

Newton's Methods

- **Advantage:**
  - More accurate local approximation of the objective,
  - The convergence is much faster.
- **Disadvantage:**
  - Need to compute the second derivatives
  - Need to compute the inverse of Hessian (time/storage consuming)

Quasi Newton's Methods

- **Main Idea:** To approximate the inverse with a matrix B_t that is iteratively refined by low rank updates to become a better approximation of $[\nabla^2 f(x_t)]^{-1}$.

Quasi Newton's Methods

- **BFGS (Broyden–Fletcher–Goldfarb–Shanno):**

Optimization Methods

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Stochastic Gradient Descent

We now minimize the *empirical risk*, m is the number of training examples.

$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x},y)\sim\hat{P}_{data}} L(f(\boldsymbol{x},\boldsymbol{\theta}),y) = \frac{1}{m}\sum_{i=1}^{m} L\left(f\left(\boldsymbol{x}^{(i)},\boldsymbol{\theta}\right),y^{(i)}\right)$$

- Optimization algorithms that use the entire training set simultaneously are called *deterministic or batch* gradient methods.

- This terminology "batch" can be somewhat confusing.
  - We use the term "batch size" to describe the size of a minibatch in the stochastic gradient descent.
  - We use the term "batch gradient descent" to imply the use of the full training set.

Stochastic Gradient Descent

- Optimization algorithms that use only a single example at a time are sometimes called *stochastic* or sometimes *online* methods.

Stochastic Gradient Descent

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- E.g., consider the cost function of leaner regression as

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

- Then we have ,

$$\begin{aligned}
\frac{\partial}{\partial\theta_j}J(\theta) &= \frac{\partial}{\partial\theta_j}\frac{1}{2}(h_\theta(x) - y)^2 \\
&= 2\cdot\frac{1}{2}(h_\theta(x) - y)\cdot\frac{\partial}{\partial\theta_j}(h_\theta(x) - y) \\
&= (h_\theta(x) - y)\cdot\frac{\partial}{\partial\theta_j}\left(\sum_{i=0}^{n}\theta_i x_i - y\right) \\
&= (h_\theta(x) - y)\, x_j
\end{aligned}$$

Batch vs Stochastic Gradient Descent

- Batch gradient descent has to scan through the entire training set before taking a single step—a costly operation if m is large.

Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}.$$

}

Batch GD

- SGD can start making progress right away, and continues to make progress with each example it looks at.
- Often, SGD gets θ "close" to the minimum much faster than batch gradient descent.

Loop {

for i=1 to m, {

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}.$$

}

}

SGD

Batch vs Stochastic Gradient Descent

- SGD may never "converge" to the minimum, and the parameters $\boldsymbol{\theta}$ will keep oscillating around the minimum of $J(\boldsymbol{\theta})$;
- But in practice most of the values near the minimum will be reasonably good approximations to the true minimum.
- Therefore, when the training set is large, SGD is often preferred over batch gradient descent.

Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}.$$

}

Batch GD

Loop {

for i=1 to m, {

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}.$$

}

}

SGD

Stochastic Gradient Descent

- Most algorithms (called *minibatch* or *minibatch stochastic* methods) fall somewhere in between, using more than one but less than all of the training examples.
- **Note**: Confusing again…… It is now common to simply call them *stochastic* methods.

Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

Require: Learning rate ϵ_k.
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{g}}$
  end while

Accelerated SGD for Deep Learning

- **Polyak's Classical Momentum** [Polyak 1964]
- **Nesterov's Momentum** [Nesterov 1983]

Polyak's Classical Momentum [Polyak 1964]

- The classical momentum (CM) accumulates an exponentially decaying moving average of past gradients and continues to move in their direction.
- Letting η be the learning rate.

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1}$$

$$\boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t} f$$

- Velocity vector $\boldsymbol{v}_t$: a memory that accumulates the directions of reduction that were chosen in the previous t steps.
- The influence of $\boldsymbol{v}$ is controlled by the *momentum coefficient* $\mu \in [0,1]$. μ is usually slightly less than 1. When $\mu = 0$:

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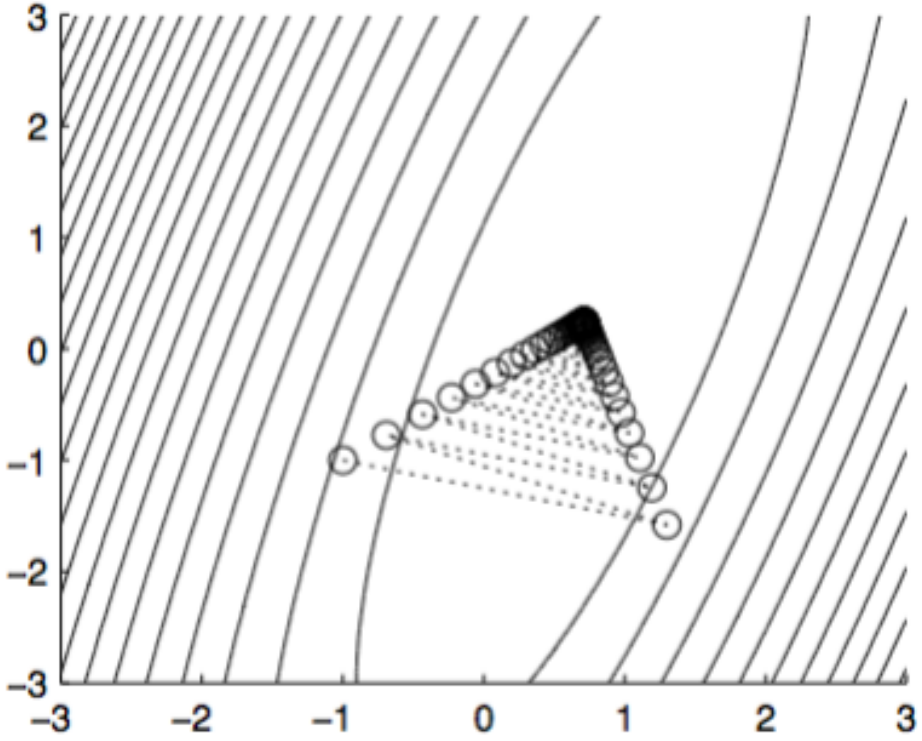
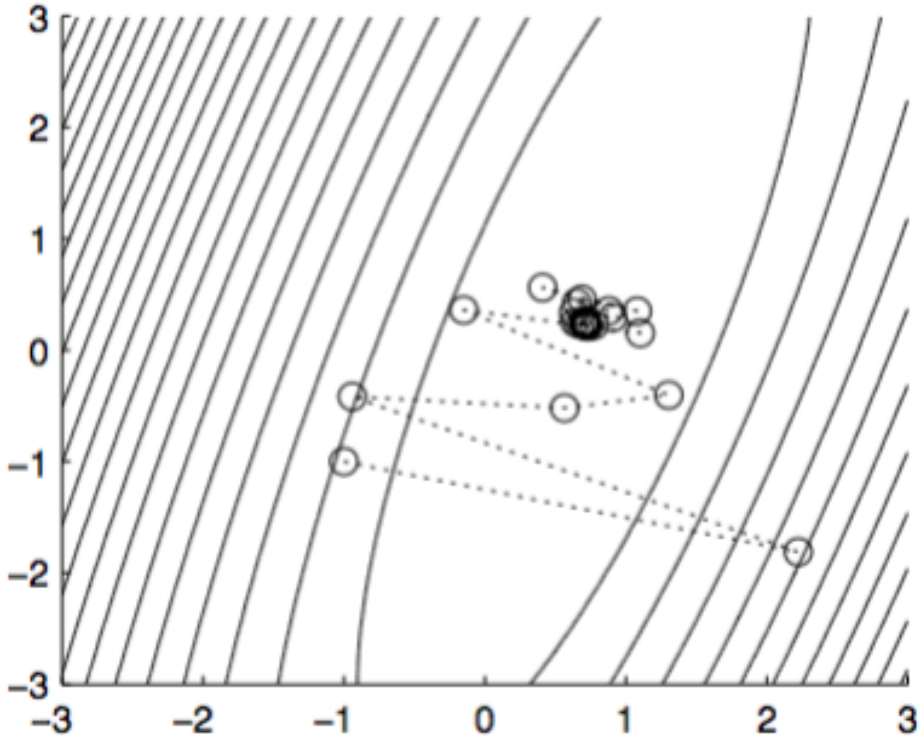
- The influence of $\boldsymbol{v}$ is controlled by the *momentum coefficient* $\mu \in [0,1]$. μ is usually slightly less than 1. When $\mu = 0$: it is just the Gradient Descent.

Polyak's Classical Momentum [Polyak 1964]

- **Motivation**: Key problem of Gradient Descent is "zig-zagging".



(a) Zig-zagging problem of GD.



(a) Trajectory of CM on same problem.

Polyak's Classical Momentum [Polyak 1964]

- The SGD algorithm with momentum is given as follows.

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1} \qquad \boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t} f$$

Algorithm 8.2 Stochastic gradient descent (SGD) with momentum

Require: Learning rate η, momentum parameter μ.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Compute velocity update: $\boldsymbol{v} \leftarrow \mu \boldsymbol{v} - \eta \boldsymbol{g}$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
  end while

Polyak's Classical Momentum [Polyak 1964]

- If the error surface is a tilted plane, the ball reaches a terminal velocity.
  - If the momentum is close to 1, this is much faster than simple gradient descent.

$$\boldsymbol{v}_\infty \to \frac{1}{1-\mu}(-\eta \nabla_{\boldsymbol{w}} f\ ) \qquad 0 < \mu < 1, \nabla_{\boldsymbol{w}_t} f \approx \nabla_{\boldsymbol{w}_{t-1}} f$$

Polyak's Classical Momentum [Polyak 1964]

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  - If the momentum is close to 1, this is much faster than simple gradient descent.

$$\boldsymbol{v}_\infty \to \frac{1}{1-\mu}(-\eta \nabla_{\boldsymbol{w}} f\ ) \qquad 0 < \mu < 1, \nabla_{\boldsymbol{w}_t} f \approx \nabla_{\boldsymbol{w}_{t-1}} f$$

$$\boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t} f = \mu(\mu \boldsymbol{v}_{t-1} - \eta \nabla_{\boldsymbol{w}_{t-1}} f) - \eta \nabla_{\boldsymbol{w}_t} f \approx \mu^{t+1} \boldsymbol{v}_0 - (\mu^t + \cdots + 1)\eta \nabla_{\boldsymbol{w}_t} f$$

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Let $S = (\mu^t + \cdots + \mu^1 + 1)$, we have,

$$\mu S + 1 = \mu(\mu^t + \cdots + \mu^1 + 1) + 1 = \mu^{t+1} + S \Rightarrow S = \frac{1-\mu^{t+1}}{1-\mu}$$

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- If $\mu = 0.99$, then can speed up ?

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- If $\mu = 0.99$, then we can speed up 100 times.

Nesterov's Accelerated Gradient [Nesterov 1983]

- The update equations of NAG are:

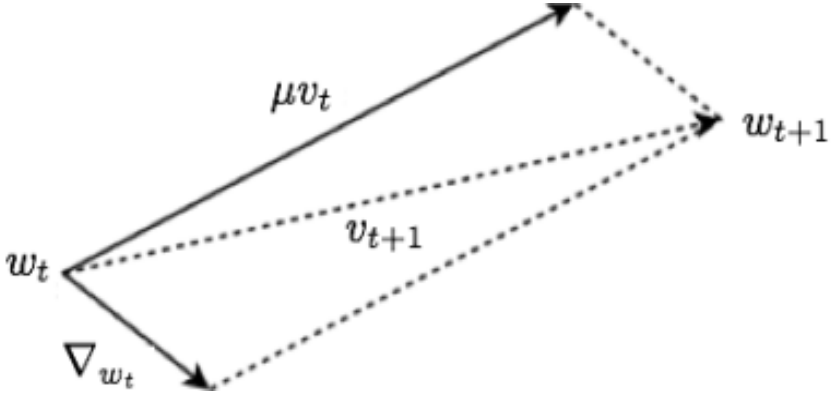
$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1}$$

$$\boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t + \mu \boldsymbol{v}_t} f$$

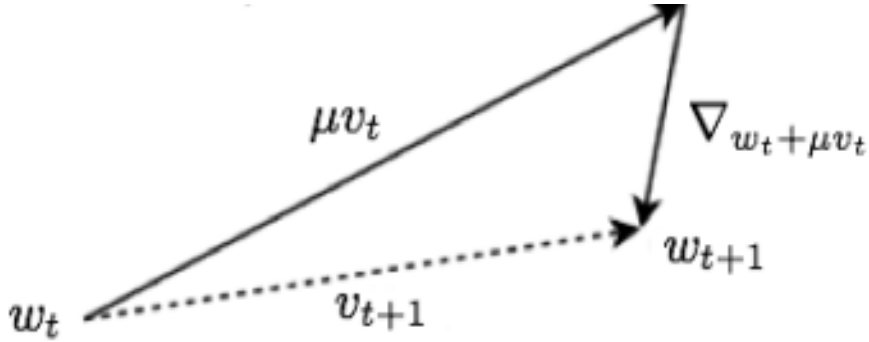
CM

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1}$$

$$\boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t} f$$



CM



NAG

Illustration of the comparison between CM and NAG.

Nesterov's Accelerated Gradient [Nesterov 1983]

- First make a big jump in the direction of the previous accumulated gradient.
- Then measure the gradient where you end up and make a correction.

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1}$$

$$\boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t + \mu \boldsymbol{v}_t} f$$

NAG

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1}$$

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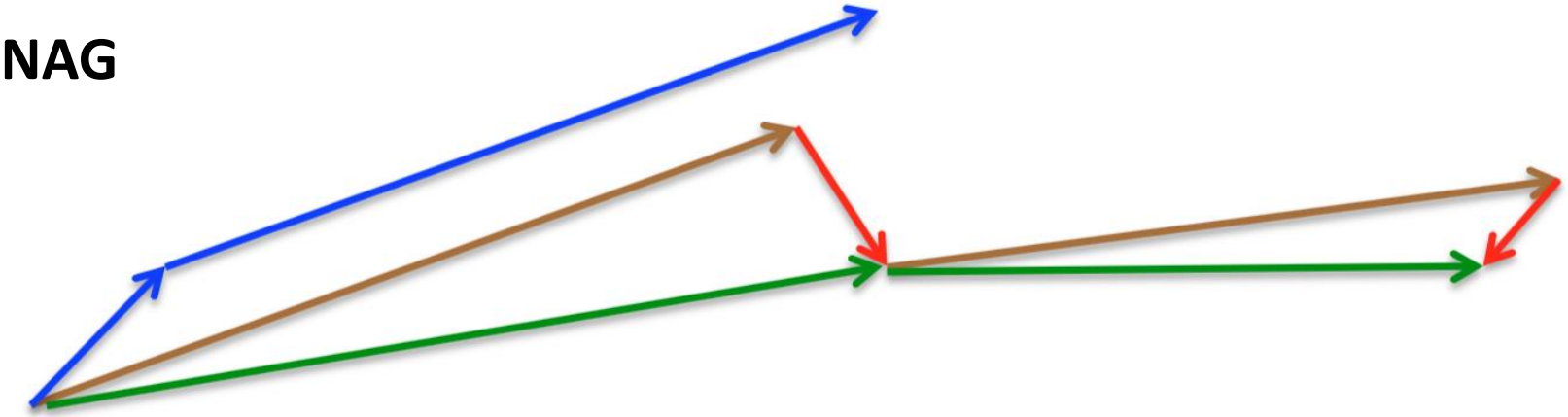
CM



brown vector = jump, red vector = correction, green vector = accumulated gradient

blue vectors = standard momentum

Nesterov's Accelerated Gradient [Nesterov 1983]

- The update equations of NAG are:

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1}$$

$$\boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t + \mu \boldsymbol{v}_t} f$$

CM

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1}$$

$$\boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t} f$$

- CM $\rightarrow$ inspecting the gradient at the current iterate of $\boldsymbol{w}_t$;
  - Faithfully trusts the current iterate;
- NAG $\rightarrow$ inspecting the gradient at $\boldsymbol{w}_t + \mu \boldsymbol{v}_t$.
  - Puts less faith into the current iterate and looks ahead in the direction suggested by the velocity vector.
- The small difference allows NAG to adapt faster and in a more stable way.

Nesterov's Accelerated Gradient [Nesterov 1983]

- The complete Nesterov momentum algorithm is presented as follows.

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \boldsymbol{v}_{t+1} \qquad \boldsymbol{v}_{t+1} = \mu \boldsymbol{v}_t - \eta \nabla_{\boldsymbol{w}_t + \mu \boldsymbol{v}_t} f$$

Algorithm 8.3 Stochastic gradient descent (SGD) with Nesterov momentum

Require: Learning rate η, momentum parameter μ.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
while stopping criterion not met **do**
Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding labels $\boldsymbol{y}^{(i)}$.
Apply interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \mu \boldsymbol{v}$
Compute gradient (at interim point): $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\tilde{\boldsymbol{\theta}}} \sum_i L(f(\boldsymbol{x}^{(i)}; \tilde{\boldsymbol{\theta}}), \boldsymbol{y}^{(i)})$
Compute velocity update: $\boldsymbol{v} \leftarrow \mu \boldsymbol{v} - \eta \boldsymbol{g}$
Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
end while

Adagrad

Adagrad (Duchi et al, COLT 2010) uses a different learning rate for every parameter θ_i at every time step t. It adapts the learning rate to the parameters.

$$g_{t,i} = \nabla_{\theta_t} J(\theta_{t,i})$$

The SGD update

$$\theta_{t+1,i} = \theta_{t,i} - \eta \cdot g_{t,i}$$

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} + \epsilon}} \cdot g_{t,i}$$

$G_t \in \mathbb{R}^{d \times d}$ is a diagonal matrix where each diagonal element i, i is the sum of the squares of the gradients w.r.t. θ_i up to time step t.

Adagrad modifies the general learning rate η at each time step t for every parameter θ_i based on the past gradients that have been computed for θ_i.

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$G_t \in \mathbb{R}^{d \times d}$ is a diagonal matrix where each diagonal element i, i is the sum of the squares of the gradients w.r.t. θ_i up to time step t.

Weakness: Since every added term is positive, the accumulated sum keeps growing which in turn causes the learning rate to shrink and eventually become infinitesimally small.

Adadelta & RMSprop

Adadelta is an extension of Adagrad that seeks to reduce its aggressive, monotonically decreasing learning rate. Instead of accumulating all past squared gradients, Adadelta restricts the window of accumulated past gradients to some fixed size *w*.

Via a decaying mechanism, $E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma) g_t^2$

RMSprop is an unpublished, adaptive learning rate method proposed by Geoff Hinton in his Coursera Class. RMSprop and Adadelta have both been developed independently around the same time to resolve Adagrad's radically diminishing learning rates.

$$E[g^2]_t = 0.9 E[g^2]_{t-1} + 0.1 g_t^2$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$$

Adam

- Adaptive Moment Estimation (Adam) is another method that computes adaptive learning rates for each parameter.
- Adam was presented by Diederik Kingma from OpenAI and Jimmy Ba from the University of Toronto in their 2015 ICLR paper (poster) titled “Adam: A Method for Stochastic Optimization“.
  1. Adam stores an exponentially decaying average of past squared gradients $\boldsymbol{v}_t$ (variance) like Adadelta and RMSprop.
  2. Adam also keeps an exponentially decaying average of past gradients $\boldsymbol{m}_t$ (mean), similar to momentum.

Adam

Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector

$m_0 \leftarrow 0$ (Initialize 1st moment vector)
$v_0 \leftarrow 0$ (Initialize 2nd moment vector)
$t \leftarrow 0$ (Initialize timestep)
while θ_t not converged **do**
  $t \leftarrow t + 1$
  $g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
  $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
  $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
  $\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
  $\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
  $\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
end while
return θ_t (Resulting parameters)

As $\boldsymbol{m_t}, \boldsymbol{v_t}$ are initialized as 0, they are biased towards 0, especially when $\beta_1 \to 1, \beta_2 \to 1$.

Summary

- **Deterministic Optimization**
  - The data for the given problem are known accurately.
  - First order method: e.g., Gradient Descent.
    - Exact Line Search
    - Inexact Line Search
      - Backtracking Line Search—Armijo Rule/Wolfe Rule
  - Second order method: e.g., Newton's method, Quasi Newton's Methods (BFGS).
- **Stochastic Optimization**
  - Using several samples of the training examples (minibatch).
  - SGD
  - SGD+Accelaration
    - Polyak's Classical Momentum
    - Nesterov's Momentum
    - Agrad/Adadelta/RMSprop/Adam

Back Up

The following slides are optional just in case that you are interested. ☺

Quasi Newton's Methods

- **BFGS (Broyden–Fletcher–Goldfarb–Shanno):**

BFGS (Broyden–Fletcher–Goldfarb–Shanno):

Main Idea: To approximate the inverse of Hessian with a matrix B_t that is iteratively refined by low rank updates to become a better approximation of $[\nabla^2 f(x_t)]^{-1}$.

- the former inverse hessian estimate $\boldsymbol{H}_n^{-1}$
- the input differences (s_n)
- the gradient differences (y_n).

QuasiNewton($f, \boldsymbol{H}_0^{-1}, x_0, QuasiUpdate$)

For n=0,1,…(until converged):

//Compute search direction and step-size

$$d = \boldsymbol{H}_0^{-1} g_n$$

$$\alpha = \min_{\alpha \geq 0} f(x_n - \alpha d)$$

$$x_{n+1} \leftarrow x_n - \alpha d$$

//store the input and gradient deltas

$$g_{n+1} = \nabla f(x_{n+1})$$

$$s_{n+1} \leftarrow x_{n+1} - x_n$$

$$y_{n+1} \leftarrow g_{n+1} - g_n$$

//update inverse hessian

$$\boldsymbol{H}_{n+1}^{-1} \leftarrow QuasiUpdate(\boldsymbol{H}_n^{-1}, s_{n+1}, y_{n+1})$$

BFGS (Broyden–Fletcher–Goldfarb–Shanno):

$$\boldsymbol{H}_{n+1}^{-1} \leftarrow QuasiUpdate(\boldsymbol{H}_{n}^{-1}, s_{n+1}, y_{n+1})$$

- What form should $QuasiUpdate$ take?
- What if we have $QuasiUpdate$ always return the identity matrix?
  - Gradient descent (The search direction is always ∇f_n).
  - This will converge to x^* for convex f.
  - This choice isn't attempting to capture second-order information about f.

Let's first think about the approximation for f near x_n:

$$p_n(\Delta x) = f(x_n) + \Delta x^T \boldsymbol{g}_n + \frac{1}{2}\Delta x^T \boldsymbol{H}_n \Delta x$$

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❑ Secant Condition

- A good property for p_n is that its gradient agrees with f at x_n and x_{n-1}, i.e.,

$$\nabla p_n(x_n) = \boldsymbol{g}_n, \qquad \nabla p_n(x_{n-1}) = \boldsymbol{g}_{n-1}$$

- Using both of the equations above:

$$\nabla p_n(x_n) - \nabla p_n(x_{n-1}) = \boldsymbol{g}_n - \boldsymbol{g}_{n-1}$$

- Using the gradient of $p_n(\cdot)$ and cancelling terms we get

$$(\boldsymbol{g}_n + \boldsymbol{H}_n x_n) - (\boldsymbol{g}_n + \boldsymbol{H}_n x_{n-1}) = (\boldsymbol{g}_n - \boldsymbol{g}_{n-1}) \Rightarrow \boldsymbol{H}_n(x_n - x_{n-1}) = (\boldsymbol{g}_n - \boldsymbol{g}_{n-1})$$

BFGS (Broyden–Fletcher–Goldfarb–Shanno):

Let's first think about the approximation for f near x_n:

$$p_n(\Delta x) = f(x_n) + \Delta x^T \boldsymbol{g}_n + \frac{1}{2}\Delta x^T \boldsymbol{H}_n \Delta x$$

❑ Secant Condition

$$\boldsymbol{H}_n \underbrace{[x_n - x_{n-1}]}_{\boldsymbol{y}_n} = \underbrace{\boldsymbol{g}_n - \boldsymbol{g}_{n-1}}_{\boldsymbol{s}_n}$$

- This ensure: $\boldsymbol{H}_{n+1}$ behaves like the Hessian at least for the difference $(x_n - x_{n-1})$.
- Assuming $\boldsymbol{H}_n$ is invertible (i.e., psd), we have,

$$\boldsymbol{H}_n^{-1}\boldsymbol{y}_n = \boldsymbol{s}_n$$

BFGS (Broyden–Fletcher–Goldfarb–Shanno):

Let's first think about the approximation for f near x_n:

$$p_n(\Delta x) = f(x_n) + \Delta x^T \boldsymbol{g}_n + \frac{1}{2}\Delta x^T \boldsymbol{H}_n \Delta x$$

❑ Symmetric Condition

- A Hessian represents the matrix of 2nd order partial derivatives;
- The Hessian is symmetric since the order of differentiation doesn't matter.

BFGS (Broyden–Fletcher–Goldfarb–Shanno):

- Given the two conditions, we take the most conservative change relative to $\boldsymbol{H}_{n-1}$,

$$\min_{\boldsymbol{H}^{-1}} \left\| \boldsymbol{H}^{-1} - \boldsymbol{H}_{n-1}^{-1} \right\|^2$$

$$\text{s.t. } \boldsymbol{H}^{-1}\boldsymbol{y}_n = \boldsymbol{s}_n$$

$\boldsymbol{H}^{-1}$ is symmetric $\quad\quad$ $\|\cdot\|$ is the Frobenius norm.

- The solution to this optimization problem is given by ,

$$\boldsymbol{H}_{n+1}^{-1} = (I - \rho_n \boldsymbol{y}_n \boldsymbol{s}_n{}^T)\boldsymbol{H}_n^{-1}(I - \rho_n \boldsymbol{s}_n \boldsymbol{y}_n{}^T) + \rho_n \boldsymbol{s}_n \boldsymbol{s}_n{}^T$$

$$\rho_n = (\boldsymbol{y}_n{}^T \boldsymbol{s}_n)^{-1}$$

- $\boldsymbol{H}_{n+1}^{-1}$ is positive definite when $\boldsymbol{H}_n^{-1}$ is.
  - We can choose any $\boldsymbol{H}_0^{-1}$ we want, including the I matrix, this is easy to ensure.

Polyak's Classical Momentum [Polyak 1964]

- Exponential decay

$$\boldsymbol{v}_{t+1} = \mu\boldsymbol{v}_t - \eta\nabla_{\boldsymbol{w}_t} f = \mu(\mu\boldsymbol{v}_{t-1} - \eta\nabla_{\boldsymbol{w}_{t-1}} f) - \eta\nabla_{\boldsymbol{w}_t} f$$

$$= \mu^{t+1}\boldsymbol{v}_0 - (\mu^t\eta\nabla_{\boldsymbol{w}_0} f + \cdots + \mu^1\eta\nabla_{\boldsymbol{w}_{t-1}} f + \eta\nabla_{\boldsymbol{w}_t} f)$$

We know that $\lim_{n\to\infty}(1+\frac{1}{n})^n = e$ $\lim_{n\to\infty}(1-\frac{1}{n})^n = \frac{1}{e}$

Let $x = \frac{1}{n} \to 0$, we have $(1-x)^{\frac{1}{x}} = \frac{1}{e}$

We 'ignore' the terms whose weights decay to less than $\frac{1}{e}$.

For example, if $\mu = 0.9$ ($x = 0.1$), to calculate $\boldsymbol{v}_{100}$, we only consider the last 10 steps (i.e., $\boldsymbol{v}_{99} \ldots \boldsymbol{v}_{90}$) as the valid memory.