AI505

Optimization

First-Order Methods

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Outline

Descent Direction Methods

How to select the descent direction?

- first-order methods that rely on gradient
- second-order methods that rely on Hessian information

Advantages of first order methods:

- cheap iterations: good for small and large scale optimization
- helpful because easy to warm restart

Limitations of first order methods:

- not hard to find challenging instances for them (instances with many saddle regions).
- can converge slowly.

Outline

Gradient Descent

The **steepest descent** direction at $\boldsymbol{x}_k$, at kth iteration of a **local descent iterative method**, is the one opposite to the gradient (**gradient descent**):

$$\boxed{\boldsymbol{d}_k = -\frac{\nabla f(\boldsymbol{x}_k)}{\|\nabla f(\boldsymbol{x}_k)\|}}$$

Guaranteed to lead to improvement if:

- f is smooth
- step size is sufficiently small
- $\boldsymbol{x}_k$ is not a stationary point (ie, $\nabla f(\boldsymbol{x}_k) = 0$)

Gradient Descent: Example

- Suppose we have

$$f(\boldsymbol{x}) = x_1 x_2^2$$

- The gradient is $\nabla f = [x_2^2, 2x_1x_2]$
- $\boldsymbol{x}_k = [1, 2]$

$$\boldsymbol{d}_{k+1} = -\frac{\nabla f(\boldsymbol{x}_k)}{\|\nabla f(\boldsymbol{x}_k)\|} = \frac{[-4, -4]}{\sqrt{16+16}} = \left[-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right]$$

Implementation

```python
class DescentMethod:
    alpha: float

class GradientDescent(DescentMethod):
    def __init__(self, f, grad, x, alpha):
        self.alpha = alpha

    def step(self, f, grad, x):
        alpha, g = self.alpha, grad(x)
        return x - alpha * g
```

Gradient Descent

Theorem: The next direction is orthogonal to the current direction.

Proof:

$$\alpha_k^* = \operatorname*{argmin}_{\alpha} f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k)$$

$$\nabla f(\boldsymbol{x}_k + \alpha_k^* \boldsymbol{d}_k) = \nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k + \alpha_k^* \boldsymbol{d}_k) = 0 \qquad \text{because } \alpha_k^* \text{ is minimum}$$

$$\nabla f(\boldsymbol{x}_k + \alpha_k^* \boldsymbol{d}_k)^T \boldsymbol{d}_k = 0 \qquad \text{because directional derivative: } \nabla_{\boldsymbol{s}} f(\boldsymbol{x}) = \nabla f(\boldsymbol{x})^T \boldsymbol{s}$$

$$\boldsymbol{d}_{k+1} = -\frac{\nabla f(\boldsymbol{x}_k + \alpha_k^* \boldsymbol{d}_k)}{\|\nabla f(\boldsymbol{x}_k + \alpha_k^* \boldsymbol{d}_k)\|} \qquad \text{gradient descent}$$

$$\boldsymbol{d}_{k+1} \cdot \boldsymbol{d}_k = -\frac{\nabla f(\boldsymbol{x}_k + \alpha_k^* \boldsymbol{d}_k)}{\|\nabla f(\boldsymbol{x}_k + \alpha_k^* \boldsymbol{d}_k)\|} \cdot \boldsymbol{d}_k = 0 \qquad \boldsymbol{d}_{k+1}^T \boldsymbol{d}_k = 0 \implies \boldsymbol{d}_{k+1} \perp \boldsymbol{d}_k$$

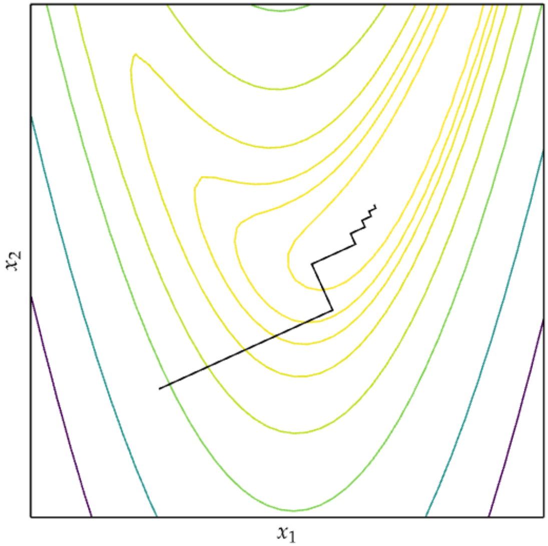
□

Gradient Descent: Example

2D Rosenbrock function

$$f(x, y) = (a - x)^2 + b(y - x^2)^2$$

Narrow valleys not aligned with gradient can be a problem



Outline

Conjugate Gradient

[Hestenes and Stiefel, 1950s]

For A symmetric positive definite:

$$A\boldsymbol{x} = \boldsymbol{b} \iff \underset{\boldsymbol{x}}{\text{minimize}}\ f(\boldsymbol{x}) \overset{def}{=} \frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x} - \boldsymbol{b}^T\boldsymbol{x}$$

$$\nabla f(\boldsymbol{x}) = A\boldsymbol{x} - \boldsymbol{b} \overset{def}{=} \boldsymbol{r}(\boldsymbol{x})$$

Conjugate Direction

Def.: A set of nonzero vectors $\{\boldsymbol{d}_0, \boldsymbol{d}_1, \ldots, \boldsymbol{d}_\ell\}$ is said to be **conjugate** with respect to the symmetric positive definite matrix A if

$$\boldsymbol{d}_i^T A \boldsymbol{d}_j = 0, \qquad \text{for all } i \neq j$$

(the vectors are linearly independent. Generally, not orthogonal.)

Theorem: Given an arbitrary $\boldsymbol{x}_0 \in \mathbb{R}^n$ and a set of conjugate vectors $\{\boldsymbol{d}_0, \boldsymbol{d}_1, \ldots, \boldsymbol{d}_{n-1}\}$ the sequence $\{\boldsymbol{x}_k\}$ generated by

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$$

where α_k is the analytical solution of $\min_{\alpha} f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k)$ given by:

$$\alpha_k = -\frac{\boldsymbol{r}_k^T \boldsymbol{d}_k}{\boldsymbol{d}_k^T A \boldsymbol{d}_k}$$

(aka, **conjugate direction algorithm**) converges to the solution $\boldsymbol{x}^*$ of the linear system and minimization problem in at most n steps.

Proof:

$$\min_{\alpha} f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k)$$

We can compute the derivative with respect to α:

$$\begin{aligned}\frac{\partial}{\partial \alpha} f(\boldsymbol{x} + \alpha \boldsymbol{d}) &= \frac{\partial}{\partial \alpha} (\boldsymbol{x} + \alpha \boldsymbol{d})^T A (\boldsymbol{x} + \alpha \boldsymbol{d}) - \boldsymbol{b}^T (\boldsymbol{x} + \alpha \boldsymbol{d}) \\ &= \boldsymbol{d}^T A (\boldsymbol{x} + \alpha \boldsymbol{d}) - \boldsymbol{d}^T \boldsymbol{b} \\ &= \boldsymbol{d}^T (A\boldsymbol{x} - \boldsymbol{b}) + \alpha \boldsymbol{d}^T A \boldsymbol{d}\end{aligned}$$

Setting $\frac{\partial f(\boldsymbol{x} + \alpha \boldsymbol{d})}{\partial \alpha} = 0$ results in:

$$\alpha_k = -\frac{\boldsymbol{d}_k^T (A\boldsymbol{x}_k - \boldsymbol{b})}{\boldsymbol{d}_k^T A \boldsymbol{d}_k} = -\frac{\boldsymbol{d}_k^T \boldsymbol{r}(\boldsymbol{x}_k)}{\boldsymbol{d}_k^T A \boldsymbol{d}_k} \qquad (1)$$

- Since the directions $\{\boldsymbol{d}_k\}$ are linearly independent, they must span the whole space $\mathbb{R}^n$. Hence, there is a set of scalars σ_k such that:

$$\boldsymbol{x}^* - \boldsymbol{x}_0 = \sigma_0 \boldsymbol{d}_0 + \sigma_1 \boldsymbol{d}_1 + \ldots + \sigma_{n-1} \boldsymbol{d}_{n-1} \qquad \text{(the ``in at most } n \text{ steps'' part)}$$

- By premultiplying this expression by $\boldsymbol{d}_k^T A$ and using the conjugacy property, we obtain:

$$\sigma_k = \frac{\boldsymbol{d}_k^T A(\boldsymbol{x}^* - \boldsymbol{x}_0)}{\boldsymbol{d}_k^T A \boldsymbol{d}_k} \tag{2}$$

- If $\boldsymbol{x}_k$ is generated by conjugate direction algorithm, then we have

$$\boldsymbol{x}_k = \boldsymbol{x}_0 + \alpha_0 \boldsymbol{d}_0 + \alpha_1 \boldsymbol{d}_1 + \ldots + \alpha_k \boldsymbol{d}_{k-1}$$

- By premultiplying this expression by $\boldsymbol{d}_k^T A$ and using the conjugacy property, we have that

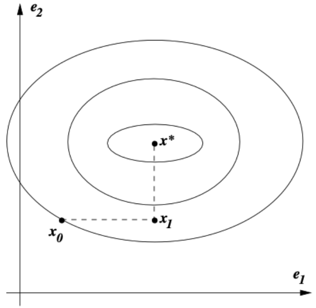
$$\boldsymbol{d}_k^T A(\boldsymbol{x}_k - \boldsymbol{x}_0) = 0$$

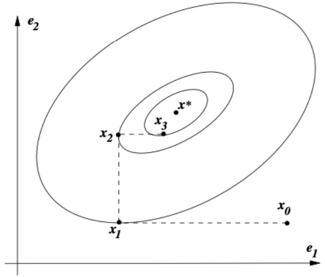
- and therefore

$$\boldsymbol{d}_k^T A(\boldsymbol{x}^* - \boldsymbol{x}_0) = \boldsymbol{d}_k^T A(\boldsymbol{x}^* - \boldsymbol{x}_k + \boldsymbol{x}_k - \boldsymbol{x}_0) = \boldsymbol{d}_k^T A(\boldsymbol{x}^* - \boldsymbol{x}_k) + \boldsymbol{d}_k^T A(\boldsymbol{x}_k - \boldsymbol{x}_0) =$$
$$= \boldsymbol{d}_k^T A(\boldsymbol{x}^* - \boldsymbol{x}_k) = \boldsymbol{d}_k^T(\boldsymbol{b} - A\boldsymbol{x}_k) = -\boldsymbol{d}_k^T \boldsymbol{r}_k.$$

- Using this result in (2) and comparing with (1) we conclude $\alpha_k = \sigma_k$. □

Interpretation of Conjugate Directions





If the matrix A is diagonal, the contours of the function $f(\cdot)$ are ellipses whose axes are aligned with the coordinate directions. In each iteration we compute one component of the optimal solution, this takes two steps in $\mathbb{R}^2$.

If A is not diagonal, its contours are elliptical, but they are usually not aligned with the coordinate directions. Finding the optimum may take more than n iterations.
Transform the problem to make A diagonal and minimize along the coordinate directions.

Transformation matrix: $S = \left[\boldsymbol{d}_0, \boldsymbol{d}_1, \ldots, \boldsymbol{d}_{n-1} \right]$

Conjugate Gradient Method

- The **conjugate gradient method** is a **first order method** with the property: In generating its set of conjugate vectors, it can compute a new vector $\boldsymbol{d}_k$ by using only the previous vector $\boldsymbol{d}_{k-1}$. Hence, little storage and computation requirements.

$$\boxed{\boldsymbol{d}_k = -\boldsymbol{r}_k + \beta_k \boldsymbol{d}_{k-1}}$$

where β_k is to be determined such that $\boldsymbol{d}_{k-1}$ and $\boldsymbol{d}_k$ must be conjugate with respect to A. By premultiplying by $\boldsymbol{d}_{k-1}^T A$ and imposing that $\boldsymbol{d}_{k-1}^T A \boldsymbol{d}_k = 0$ we find that

$$\beta_k = \frac{\boldsymbol{r}_k^T A \boldsymbol{d}_{k-1}}{\boldsymbol{d}_{k-1}^T A \boldsymbol{d}_{k-1}}$$

- Larger values of β indicate that the previous descent direction contributes more strongly.
- $\boldsymbol{d}_0$ is commonly chosen to be the steepest descent direction at $\boldsymbol{x}_0$
- Advantage with respect to steepest descent: implicitly reuses previous information about the function and thus better convergence.

Algorithm CG

Basic version:

```
Input: $f, \boldsymbol{x}_0$
Output: $x^*$
Set $\boldsymbol{r}_0 \leftarrow A\boldsymbol{x}_0 - b, \boldsymbol{d}_0 \leftarrow \boldsymbol{r}_0, k \leftarrow 0$;
while $\boldsymbol{r}_k \neq 0$ do
    $\alpha_k \leftarrow -\frac{\boldsymbol{d}_k^T \boldsymbol{r}(\boldsymbol{x}_k)}{\boldsymbol{d}_k^T A \boldsymbol{d}_k}$;
    $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$;
    $\boldsymbol{r}_{k+1} \leftarrow A\boldsymbol{x}_{k+1} - \boldsymbol{b}$;
    $\beta_{k+1} \leftarrow \frac{\boldsymbol{r}_{k+1}^T A \boldsymbol{d}_k}{\boldsymbol{d}_k^T A \boldsymbol{d}_k}$;
    $\boldsymbol{d}_{k+1} \leftarrow -\boldsymbol{r}_{k+1} + \beta_{k+1} \boldsymbol{d}_k$;
    $k \leftarrow k + 1$;
```

Computationally improved version:

```
Input: $f, \boldsymbol{x}_0$
Output: $x^*$
Set $\boldsymbol{r}_0 \leftarrow A\boldsymbol{x}_0 - b, \boldsymbol{d}_0 \leftarrow \boldsymbol{r}_0, k \leftarrow 0$;
while $\boldsymbol{r}_k \neq 0$ do
    $\alpha_k \leftarrow -\frac{\boldsymbol{r}(\boldsymbol{x}_k)^T \boldsymbol{r}(\boldsymbol{x}_k)}{\boldsymbol{d}_k^T A \boldsymbol{d}_k}$;
    $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$;
    $\boldsymbol{r}_{k+1} \leftarrow \boldsymbol{r}_k + \alpha_k A \boldsymbol{d}_k$;
    $\beta_{k+1} \leftarrow \frac{\boldsymbol{r}_{k+1}^T \boldsymbol{r}_{k+1}}{\boldsymbol{r}_k^T \boldsymbol{r}_k}$;
    $\boldsymbol{d}_{k+1} \leftarrow -\boldsymbol{r}_{k+1} + \beta_{k+1} \boldsymbol{d}_k$;
    $k \leftarrow k + 1$;
```

- we never need to know the vectors $\boldsymbol{x}, \boldsymbol{r}$, and $\boldsymbol{d}$ for more than the last two iterations.
- major computational tasks: the matrix–vector product $A\boldsymbol{d}_k$, inner products $\boldsymbol{d}_k^T A \boldsymbol{d}_k$ and $\boldsymbol{r}_{k+1}^T \boldsymbol{r}_{k+1}$, and three vector sums

NonLinear Conjugate Gradient Methods

- The conjugate gradient method can be applied to nonquadratic functions as well.
- Smooth, continuous functions behave like quadratic functions close to a local minimum
- but! we do not know the value of A that best approximates f around $\boldsymbol{x}_k$. Instead, several choices for β_k tend to work well
- Two changes:
  - α_k is computed by solving an approximate line search
  - the residual $\boldsymbol{r}$, (it was simply the gradient of f), must be replaced by the gradient of the nonlinear objective f.

NonLinear Conjugate Gradient Methods

Fletcher-Reeves Method:

```
Input: $f, \boldsymbol{x}_0$
Output: $x^*$
Evaluate $f_0 = f(\boldsymbol{x}_0), \nabla f_0 = \nabla f(\boldsymbol{x}_0)$;
Set $\boldsymbol{d}_0 \leftarrow -\nabla f_0$, $k \leftarrow 0$;
while $\nabla f_k \neq 0$ do
    Compute $\alpha_k$ by line search and set
     $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$;
    Evaluate $\nabla f_{k+1}$;
    $\beta_{k+1}^{FR} \leftarrow \frac{\nabla f_{\mathbf{k+1}}^T \nabla f_{\mathbf{k+1}}}{\nabla f_k^T \nabla f_k}$;
    $\boldsymbol{d}_{k+1} \leftarrow -\nabla f_{k+1} + \beta_{k+1}^{FR} \boldsymbol{d}_k$;
    $k \leftarrow k+1$;
```

Polak-Ribière:

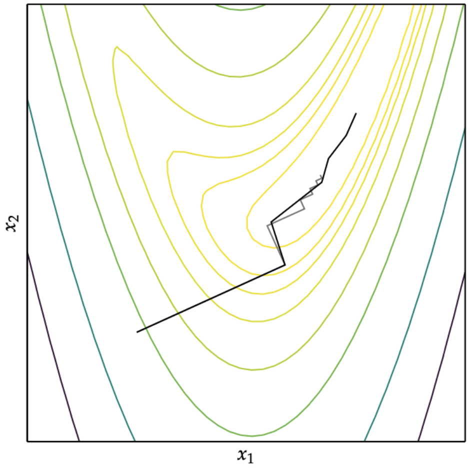
```
Input: $f, \boldsymbol{x}_0$
Output: $x^*$
Evaluate $f_0 = f(\boldsymbol{x}_0), \nabla f_0 = \nabla f(\boldsymbol{x}_0)$;
Set $\boldsymbol{d}_0 \leftarrow -\nabla f_0$, $k \leftarrow 0$;
while $\nabla f_k \neq 0$ do
    Compute $\alpha_k$ by line search and set
     $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$;
    Evaluate $\nabla f_{k+1}$;
    $\beta_{k+1}^{PR} \leftarrow \frac{\nabla f_{\mathbf{k+1}}^T (\nabla f_{\mathbf{k+1}} - \nabla f_k)}{\nabla f_k^T \nabla f_k}$;
    $\boldsymbol{d}_{k+1} \leftarrow -\nabla f_{k+1} + \beta_{k+1}^{PR} \boldsymbol{d}_k$;
    $k \leftarrow k+1$;
```

PR with:

$$\beta_{k+1}^{+} = \max\{\beta_{k+1}^{PR}, 0\}$$

becomes PR^{+} and guaranteed to converge (satisfies first Wolfe conditions).

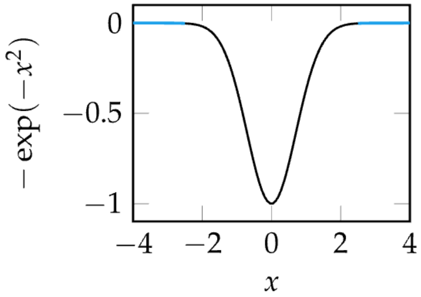
The conjugate gradient method with the Polak-Ribière update. Gradient descent is shown in gray.



Outline

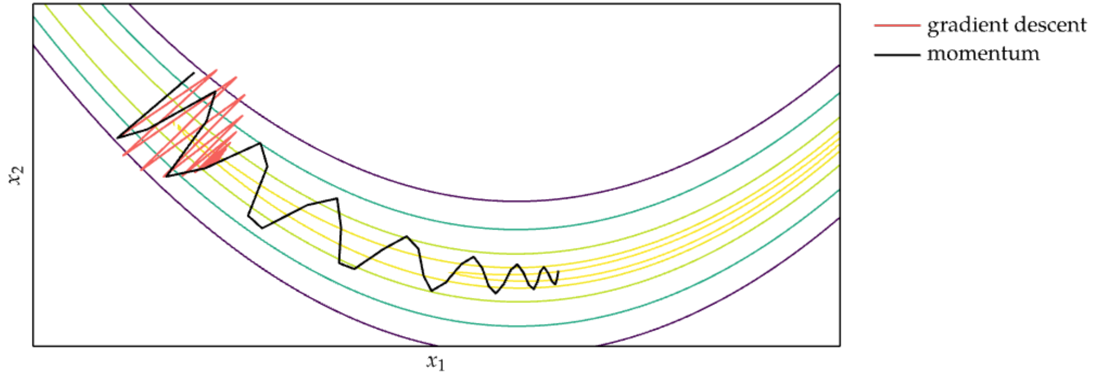
Accelerated Descents

- Addresses common convergence issues
- Some functions have regions with very small gradients (flat surface) where gradient descent gets stuck



Momentum

Rosenbrock function with $b = 100$



Momentum overcomes these issues by replicating the effect of physical momentum

Momentum

Momentum update equations:

$$\boxed{\begin{aligned} \mathbf{v}_{k+1} &= \beta \mathbf{v}_k - \alpha \nabla f(\mathbf{x}_k) \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \mathbf{v}_{k+1} \end{aligned}}$$

```python
import numpy as np

class Momentum(DescentMethod):
  alpha: float # learning rate
  beta: float # momentum decay
  v: np.array # momentum

  def __init__(self, alpha, beta, f, grad, x):
    self.alpha = alpha
    self.beta = beta
    self.v = np.zeros_like(x)

  def step(self, grad, x):
    self.v = self.beta * self.v - self.alpha * ↪
        ↪grad(x)
    return x + self.v
```

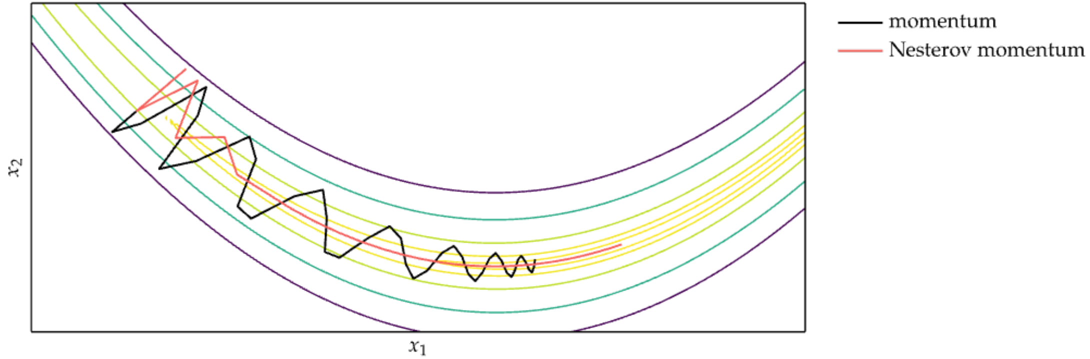
Nesterov Momentum

Issue of momentum: steps do not slow down enough at the bottom of a valley, overshoot.

Nesterov Momentum update equations:

$$\boldsymbol{v}_{k+1} = \beta \boldsymbol{v}_k - \alpha \nabla f(\boldsymbol{x}_k + \beta \boldsymbol{v}_k)$$

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{v}_{k+1}$$



Adagrad

- Instead of using the same learning rate for all components of $\boldsymbol{x}$, **Adaptive Subgradient method** (Adagrad) adapts the learning rate for each component of $\boldsymbol{x}$. For each component of $\boldsymbol{x}$, the update equation is

  $$x_{i,k+1} = x_{i,k} - \frac{\alpha}{\epsilon + \sqrt{s_{i,k}}} \nabla f_i(\boldsymbol{x}_k)$$

  where

  $$s_{i,k} = \sum_{j=1}^{k} \left(\nabla f_i(\boldsymbol{x}_j)\right)^2$$

  $$\epsilon \approx 1 \times 10^{-8}, \alpha = 0.01$$

- components of $\boldsymbol{s}$ are strictly nondecreasing, hence learning rate decreases over time

RMSProp

- Extends Adagrad to avoid monotonically decreasing learning rate by maintaining a decaying average of squared gradients

$$\hat{s}_{k+1} = \gamma \hat{s}_k + (1-\gamma)\left(\nabla f_(\boldsymbol{x}_k) \odot \nabla f(\boldsymbol{x}_k)\right), \qquad \gamma \in [0,1], \qquad \odot \text{ element-wise product}$$

Update Equation

$$\begin{aligned} x_{i,k+1} &= x_{i,k} - \frac{\alpha}{\epsilon + \sqrt{\hat{s}_{i,k}}} \nabla f_i(\boldsymbol{x}_k) \\ &= x_{i,k} - \frac{\alpha}{\epsilon + RMS(\nabla f_i(\boldsymbol{x}_k))} \nabla f_i(\boldsymbol{x}_k) \end{aligned}$$

root mean square: For n values $\{x_1, x_2, \ldots, x_n\}$

$$x_{\text{RMS}} = \sqrt{\frac{1}{n}\left({x_1}^2 + {x_2}^2 + \cdots + {x_n}^2\right)}.$$

AdaDelta

Also extends Adagrad to avoid monotonically decreasing learning rate
Modifies RMSProp to eliminate learning rate parameter entirely

$$x_{i,k+1} = x_{i,k} - \frac{RMS(\Delta x_i)}{\epsilon + RMS(\nabla f_i(\boldsymbol{x}))} \nabla f_i(\boldsymbol{x}_k)$$

Adam

- The **adaptive moment estimation method** (Adam), adapts the learning rate to each parameter.
- stores both an exponentially decaying gradient like momentum and an exponentially decaying squared gradient like RMSProp and Adadelta
- At each iteration, a sequence of values are computed

$$\begin{aligned}
\text{Biased decaying momentum} \quad & \boldsymbol{v}_{k+1} = \beta \boldsymbol{v}_k - \alpha \nabla f(\boldsymbol{x}_k) \\
\text{Biased decaying squared gradient} \quad & \boldsymbol{s}_{k+1} = \gamma \boldsymbol{s}_k + (1-\gamma)\left(\nabla f(\boldsymbol{x}_k) \odot \nabla f(\boldsymbol{x}_k)\right) \\
\text{Corrected decaying momentum} \quad & \hat{v}_{k+1} = \boldsymbol{v}_{k+1}/(1-\gamma_{v,k}) \\
\text{Corrected decaying squared gradient} \quad & \hat{s}_{k+1} = \boldsymbol{s}_{k+1}/(1-\gamma_{s,k}) \\
\text{Next iterate} \quad & \boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha \hat{v}_{k+1}/(\epsilon + \sqrt{\hat{s}_{k+1}})
\end{aligned}$$

- Defaults: $\alpha = 0.001, \gamma_v = 0.9, \gamma_s = 0.999, \epsilon = 1 \times 10^{-8}$

Adamax

Same as Adam, but based on the max-norm L_∞.

$$\begin{aligned} \boldsymbol{s}_{k+1} &= \gamma^\infty \boldsymbol{s}_k + (1-\gamma^\infty)\left(\|\nabla f(\boldsymbol{x}_k)\|_\infty\right) \\ &= \max\left(\gamma \boldsymbol{s}_k, \|\nabla f(\boldsymbol{x}_k)\|_\infty\right) \end{aligned}$$

Nadam

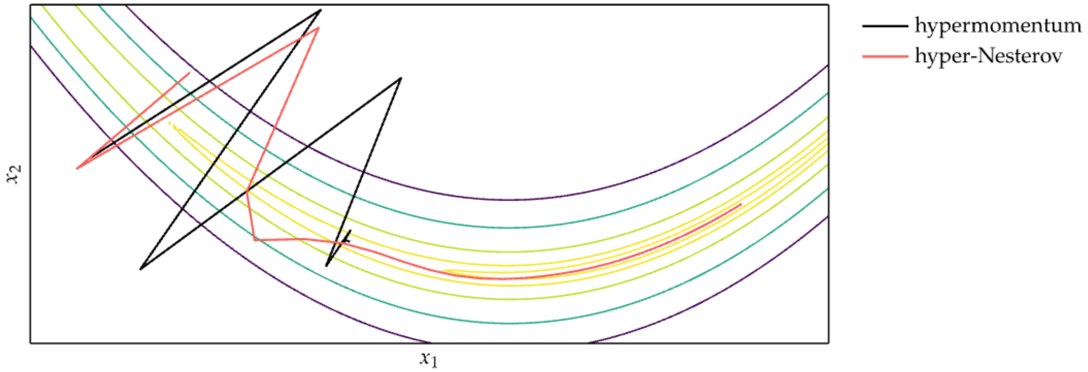
Nadam

- Nesterov-accelerated Adaptive Moment Estimation
- Adam is basically RMSProp with momentum
- We have seen that Nesterov is often more efficient
- Welcome to Nadam: Adam which uses the Nesterov momentum.

Hypergradient Descent

- Learning rate determines how sensitive the method is to the gradient signal.
- Many accelerated descent methods are highly sensitive to hyperparameters such as learning rate.
- Applying gradient descent to a hyperparameter of an underlying descent method is called hypergradient descent
- Requires computing the partial derivative of the objective function with respect to the hyperparameter

Hypergradient Descent



Summary

- Gradient descent follows the direction of steepest descent.
- The conjugate gradient method can automatically adjust to local valleys.
- Descent methods with momentum build up progress in favorable directions.
- A wide variety of accelerated descent methods use special techniques to speed up descent.
- Hypergradient descent applies gradient descent to the learning rate of an underlying descent method.