04 Numerical Optimization

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Information: *Brief introduction to gradient descent, how gradient descent is supported in pytorch, convex functions, and some numerical considerations to kept in mind*

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1 Gradient Descent Optimization

1.1 Motivation

- Most ML/DL algorithms involve **optimization** of some sort.
  - Optimization refers to the task of either **minimizing** or maximizing some function $f(\mathbf{x})$ by altering $\mathbf{x}$
  - Usually phrase most optimization problems in terms of minimizing $f(\mathbf{x})$
  - Maximization may be accomplished via s minimization algorithm by minimizing $-f(\mathbf{x})$
- Usually the function we want to minimize is called the **objective function**, or **criterion**. In ML/DL contexts, the name **loss function** is often used.
  - As mentioned in introduction, a loss function quantifies the *distance* between the **real** and **predicted** value of the target.
  - Usually be a non-negative number where smaller values are better and perfect predictions incur a loss of 0
  - Usually denoted as $L(\boldsymbol{\theta})$ where $\boldsymbol{\theta}$ is usually the parameter of ML/DL models
- Usually denote the value that minimizes a function with a superscript $*$
  - $\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\text{argmin}} L(\boldsymbol{\theta})$
- Most ML/DL algorithms are so complex that it is difficult or impossible to find the closed form solution for the optimization problem
  - Use numerical optimization method instead
- One common algorithm is **gradient descent**, other optimization algorithms are
  - Expectation Maximization
  - Sampling-based optimization
  - Greedy optimization

1.2 Definition

- **Definition**:
  - A **first-order iterative** optimization algorithm for finding **local minimum** of a **differential** function.

    * The idea is to take **repeated steps** in the opposite direction of the **gradient** of the function at the current point, because this is the direction of steepest descent.
    * As it calculates the **first-order** derivative, it requires the objective function to be **differential**
    * Converge when first-order derivative is zero, which only ensures reaching **local minimum** for general functions
- **Theory**:
  - Based on the observation that if the multi-variable function $F(\mathbf{x})$ is defined and differentiable in a neighborhood of a point $\mathbf{a}$, then $F(\mathbf{x})$ decreases **fastest** if one goes from $\mathbf{a}$ in the direction of the negative gradient of F at $\mathbf{a}$, which is $-\nabla F(\mathbf{a})$. It follows that if

    $$\mathbf{a}_{n+1} = \mathbf{a}_n - \gamma \nabla F(\mathbf{a}_n)$$

    for a $\gamma \in \mathbb{R}_+$ small enough, then

    $$F(\mathbf{a}_n) \geq F(\mathbf{a}_{n+1})$$

- Simple form of **vanilla gradient descent** (GD):
  1. Start at random parameter $\boldsymbol{\theta}$
  2. Repeat until converged
     - $\mathbf{d} \leftarrow -\nabla L(\boldsymbol{\theta})$
     - $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \mathbf{d}^T$
  - α is called **learning rate** or **step size**

1.3 Select appropriate learning rate

- Too large α leads to instability and even divergence
- Too small α leads to slow convergence
- **Steepest gradient descent** use line search to compute the best α
  1. Start at random parameter $\boldsymbol{\theta}$
  2. Repeat until converged
     - $\mathbf{d} \leftarrow -\nabla L(\boldsymbol{\theta})$
     - $\alpha^* \leftarrow \underset{\alpha}{\operatorname{argmin}}\{L(\boldsymbol{\theta} + \alpha \mathbf{d}^T)\}$
     - $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha^* \mathbf{d}^T$
- **Adaptive learning rates** may help, but not always
  - $\alpha = \frac{1}{t}$, approaches 0 but can cover an infinite distance since $\lim_{a \to \infty} \sum_{t=1}^{a} \frac{1}{t} = \infty$
- **Coordinate Descent** update one parameter at a time
  - Removes problem of selecting step size
  - Each update can be very fast, but lots of updates

1.4 Slow convergence due to Poor Conditioning

- **Conditioning** refers to how rapidly a function changes with respect to small changes in its inputs.
- Consider the function

  $$f(x) = \mathbf{A}^{-1}\mathbf{x}$$

  When $\mathbf{A} \in \mathbb{R}^{n \times n}$ has an eigenvalue decomposition, its **condition number** is

  $$\max_{i,j} \left| \frac{\lambda_i}{\lambda_j} \right|$$

This is the ratio of the magnitude of the largest and smallest eigenvalue

- A problem with a **low condition number** is said to be **well-conditioned**, while a problem with a high condition number is said to be ill-conditioned
  - In non-mathematical terms, an ill-conditioned problem is one where, for a small change in the inputs there is a large change in the answer or dependent variable, which means the correct solution to the equation becomes hard to find
  - Condition number is a property of the problem
- **Gradient descent** is very sensitive to **condition number** of the problem
  - No good choice of step size. Tiny change in one variable could lead to great change in dependent variable.
- **Solutions:**
  - **Newton's method:** Correct for local second derivative. (Sphere the ellipse)
    - Too much computation and too difficult to implement
  - **Alternative methods**:
    - Preconditioning: Easy, but tends to be ad-hoc, not so robust
    - Momentum

1.5 Compute Loss Gradient

- Take the **mean square error** as an example:

$$\begin{aligned}\nabla_{\boldsymbol{\theta}} L_{MSE}(\boldsymbol{\theta}) &= \nabla_{\boldsymbol{\theta}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \left\| \mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i) \right\|^2 \right\} \\ &= \frac{1}{N} \sum_{i=1}^{N} \nabla_{\boldsymbol{\theta}} \left\{ (\mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i))^T (\mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i)) \right\}\end{aligned}$$

  Use the chain rule and scale-by-vector matrix calculus identity that

$$\frac{\partial \mathbf{x}^T \mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{x}^T$$

  We can get

$$\begin{aligned}\nabla_{\boldsymbol{\theta}} L_{MSE}(\boldsymbol{\theta}) &= \frac{2}{N} \sum_{i=1}^{N} (\mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i))^T \nabla_{\boldsymbol{\theta}} (\mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i)) \\ &= \frac{2}{N} \sum_{i=1}^{N} (\mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i))^T \nabla_{\boldsymbol{\theta}} (-f_{\boldsymbol{\theta}}(\mathbf{x}_i)) \\ &= -\frac{2}{N} \sum_{i=1}^{N} (\mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i))^T \nabla_{\boldsymbol{\theta}} (f_{\boldsymbol{\theta}}(\mathbf{x}_i))\end{aligned}$$

- The result of the gradient usually includes three parts:
  - Sum over training data. It consists of a lot of computations but the way of computation is relatively easy and straight forward
  - Prediction error term such as $\mathbf{y}_i - f_{\boldsymbol{\theta}}(\mathbf{x}_i)$ in MSE, which is usually easy to get
  - Gradient of inference function $\nabla_{\boldsymbol{\theta}}(f_{\boldsymbol{\theta}}(\mathbf{x}_i))$, which is difficult to solve
    - Enabled by automatic differentiation built into modern domain specific languages such as Pytorch, Tensorflow, …
    - For neural networks, this is known as **back propagation**

2 Automatic Differentiation via Pytorch

2.1 Data Manipulation via Pytorch

- The n-dimensional array is usually called the tensor
- *tensor* class in Pytorch is similar to *NumPy*'s *ndarray* with several additional features
  - GPU is well-supported to accelerate the computation whereas *NumPy* only supports CPU computation
  - *tensor* class supports automatic differentiation
- The Pytorch documentation shows the full attributes

2.1.1 Create a tensor

- To get started, import **torch**. Although it's called Pytorch, we should import **torch** instead of pytorch

[1]:
```
import torch
# Check the version of a module
print(torch.__version__)
```

```
1.8.1
```

- Common ways to creating a tensor
  - torch.arange(start,end,step)
  - torch.zeros(shape)
  - torch.ones(shape)
  - torch.randn(shape)
  - torch.tensor(elements)

[2]:
```
torch.arange(0, 12, 1)
```

[2]:
```
tensor([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11])
```

[3]:
```
torch.zeros((3, 4))
```

[3]:
```
tensor([[0., 0., 0., 0.],
        [0., 0., 0., 0.],
        [0., 0., 0., 0.]])
```

[4]:
```
torch.ones((2, 5))
```

[4]:
```
tensor([[1., 1., 1., 1., 1.],
        [1., 1., 1., 1., 1.]])
```

[5]:
```
torch.randn(10)
```

[5]:
```
tensor([ 0.1833, -1.4853, -2.6226,  1.3522, -0.7521,  1.5946,  1.5680, -0.4013,
        -1.8723, -1.3914])
```

[6]:
```
torch.tensor([[1, 2, 3], [4, 5, 6]])
```

[6]:
```
tensor([[1, 2, 3],
        [4, 5, 6]])
```

- One can access a tensor's shape by viewing the **shape** attribute

[7]:
```
torch.ones((4, 5)).shape
```

[7]:
```
torch.Size([4, 5])
```

- **reshape** method can change the shape of a tensor without altering either the number of elements or their values.
  - No need to manually specify every dimension
  - Can place -1 for the dimension that we would like tensors to automatically infer

[8]:
```
torch.arange(12).reshape(3, 4)
```

[8]:
```
tensor([[ 0,  1,  2,  3],
        [ 4,  5,  6,  7],
        [ 8,  9, 10, 11]])
```

[9]:
```
torch.arange(12).reshape(3, -1)
```

[9]:
```
tensor([[ 0,  1,  2,  3],
        [ 4,  5,  6,  7],
        [ 8,  9, 10, 11]])
```

2.1.2 Type of a tensor

- Usually, a tensor is created as **tensor.float32** (32-bit floating point) by default. One can view its type in the **dtype** attribute
  - When creating a tensor using **torch.tensor**, tensor with all integers would be created as **torch.int64** (64-bit signed integer)
- Full tensor types can be viewed in the documentation

[10]:
```
torch.ones(10).dtype
```

[10]:
```
torch.float32
```

[11]:
```
torch.tensor([[1, 2, 3], [4, 5, 6]]).dtype
```

[11]:
```
torch.int64
```

[12]:
```
# Only add one dot after the first element
torch.tensor([[1., 2, 3], [4, 5, 6]]).dtype
```

[12]:
```
torch.float32
```

- One can assign the wanted type when creating the tensor by setting the **dtype** attribute to
  - *torch.float32*, 32-bit floating point
  - *torch.float64*, 64-bit floating point

  - *torch.uint8*, 8-bit unsigned integer
  - *torch.int8*, 8-bit signed integer
  - *torch.int32*, 32-bit signed integer
  - *torch.int64*, 64-bit signed integer
  - *torch.bool*, Boolean

[13]:
```
torch.ones(10, dtype=torch.float64).dtype
```

[13]:
```
torch.float64
```

[14]:
```
torch.ones(10, dtype=torch.uint8).dtype
```

[14]:
```
torch.uint8
```

[15]:
```
torch.ones(10, dtype=torch.int32).dtype
```

[15]:
```
torch.int32
```

- One can also construct the type of a tensor from list or numpy array using the method:
  - *FloatTensor*, 32-bit floating point
  - *DoubleTensor*, 64-bit floating point
  - *ByteTensor*, 8-bit unsigned integer
  - *CharTensor*, 8-bit signed integer
  - *IntTensor*, 32-bit signed integer
  - *LongTensor*, 64-bit signed integer
  - *BoolTensor*, Boolean

[16]:
```
torch.DoubleTensor([1, 2, 3]).dtype
```

[16]:
```
torch.float64
```

[17]:
```
torch.ByteTensor([1, 2, 3]).dtype
```

[17]:
```
torch.uint8
```

2.1.3 Use GPU for tensor computation

- Unless otherwise specified, a new tensor will be stored in main memory and designated for CPU-based computation
- One can check which device the tensor is designated for by viewing the **device** attribute

[18]:
```
torch.ones(10).device
```

[18]:
```
device(type='cpu')
```

- One can always set the create a device if a GPU supporting cuda is available and use **to(device)** method to determine the device on which a tensor is or will be allocated
  - Assign the **device** parameter when creating a tensor also works

[19]:
```
cuda0 = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
cuda0
```

[19]:
```
device(type='cuda', index=0)
```

[20]:
```
torch.ones(5, device=cuda0)
```

[20]:
```
tensor([1., 1., 1., 1., 1.], device='cuda:0')
```

[21]:
```
# If available, indexing the cuda also works
torch.ones(5, device=0)
```

[21]:
```
tensor([1., 1., 1., 1., 1.], device='cuda:0')
```

[22]:
```
# If avaiable, the string also works
torch.ones(5, device="cuda:0")
```

[22]:
```
tensor([1., 1., 1., 1., 1.], device='cuda:0')
```

[23]:
```
# Use the to method the move a tensor
x = torch.ones(5).to(cuda0)
x
```

[23]:
```
tensor([1., 1., 1., 1., 1.], device='cuda:0')
```

[24]:
```
# One can also move a tensor from GPU to CPU
x.to("cpu").device
```

[24]:
```
device(type='cpu')
```

2.1.4 Operations

- Common standard arithmetic operators have all been lifted to element-wise operations

[25]:
```
x = torch.tensor([1., 2., 4., 8.])
c = 1.
x + c, x * c, x**c
```

[25]:
```
(tensor([2., 3., 5., 9.]), tensor([1., 2., 4., 8.]), tensor([1., 2., 4., 8.]))
```

[26]:
```
x = torch.tensor([1., 2., 4., 8.])
y = torch.tensor([4., 3., 2., 1.])
x + y, x * y, x**y
```

[26]:
```
(tensor([5., 5., 6., 9.]),
 tensor([4., 6., 8., 8.]),
 tensor([ 1.,  8., 16.,  8.]))
```

[27]:
```
torch.exp(x)
```

[27]:
```
tensor([2.7183e+00, 7.3891e+00, 5.4598e+01, 2.9810e+03])
```

- Matrix multiplication is also supported

[28]:
```
A = torch.randn((4, 3))
B = torch.randn((3, 5))
# Two ways of matrix multiplication
torch.mm(A, B), A @ B
```

[28]:
```
(tensor([[ 1.7055, -0.0886,  1.8231,  1.7564, -2.7292],
         [-2.0987, -0.2093, -2.1729, -1.9152,  1.6844],
         [ 0.1432,  0.4736,  0.6370, -0.4225, -2.1120],
         [-0.5778,  0.4198, -0.0482, -1.1163, -1.9259]]),
 tensor([[ 1.7055, -0.0886,  1.8231,  1.7564, -2.7292],
         [-2.0987, -0.2093, -2.1729, -1.9152,  1.6844],
         [ 0.1432,  0.4736,  0.6370, -0.4225, -2.1120],
         [-0.5778,  0.4198, -0.0482, -1.1163, -1.9259]]))
```

[29]:
```
A = torch.randn((5, 4))
B = torch.randn((5, 4))
# Two ways of elementwise multiplication
torch.mul(A, B), A * B
```

[29]:
```
(tensor([[-0.0949, -1.5523, -0.2367,  0.4972],
         [-0.4520,  0.1967, -0.0363,  0.3360],
         [ 1.0668, -0.3951, -0.1567, -0.3507],
         [ 0.3363,  0.1538, -0.0893,  0.0107],
         [ 0.5939, -0.9762, -0.0580,  0.1045]]),
 tensor([[-0.0949, -1.5523, -0.2367,  0.4972],
         [-0.4520,  0.1967, -0.0363,  0.3360],
         [ 1.0668, -0.3951, -0.1567, -0.3507],
         [ 0.3363,  0.1538, -0.0893,  0.0107],
         [ 0.5939, -0.9762, -0.0580,  0.1045]]))
```

- We can also **concatenate** multiple tensors together, stacking them end-to-end to form a larger tensor. We just need to provide a list of tensors and tell the system along which axis to concatenate.

[30]:
```
A = torch.arange(0, 12, 1).reshape((3, 4))
B = torch.ones((3, 4))
# dim stands for the index of dimension in which the tensors are concatenated
torch.cat((A, B), dim=0), torch.cat((A, B), dim=1)
```

[30]:
```
(tensor([[ 0.,  1.,  2.,  3.],
         [ 4.,  5.,  6.,  7.],
         [ 8.,  9., 10., 11.],
         [ 1.,  1.,  1.,  1.],
         [ 1.,  1.,  1.,  1.],
         [ 1.,  1.,  1.,  1.]]),
```

```
tensor([[ 0.,  1.,  2.,  3.,  1.,  1.,  1.,  1.],
        [ 4.,  5.,  6.,  7.,  1.,  1.,  1.,  1.],
        [ 8.,  9., 10., 11.,  1.,  1.,  1.,  1.]]))
```

- Also, we can construct a binary tensor via logical statements

[31]:
```
A = torch.arange(0, 12, 1).reshape((3, 4))
B = 5 * torch.ones((3, 4))
A == B, A > B
```

[31]:
```
(tensor([[False, False, False, False],
         [False,  True, False, False],
         [False, False, False, False]]),
 tensor([[False, False, False, False],
         [False, False,  True,  True],
         [ True,  True,  True,  True]]))
```

2.1.5 Broadcasting Mechanism

- Under certain conditions, even shapes differ, we can still perform **element-wise** operations by invoking the **broadcasting mechanism**.
  - First, expand one or both arrays by copying elements appropriately so that after this transformation, the two tensors have the same shape.
  - Second, carry out the element-wise operation on the resulting arrays
- In most cases, we broadcast along an axis where an array initially only has length 1

[32]:
```
a = torch.arange(3).reshape(3, 1)
b = torch.arange(2).reshape(1, 2)
a, b, a + b
```

[32]:
```
(tensor([[0],
         [1],
         [2]]),
 tensor([[0, 1]]),
 tensor([[0, 1],
         [1, 2],
         [2, 3]]))
```

2.1.6 Indexing and Slicing

- As in standard Python lists, we can access elements according to their relative position to the end of the list by using negative indices

[33]:
```
X = torch.arange(16).reshape(4, 4)
X, X[-1], X[1:3]
```

[33]:
```
(tensor([[ 0,  1,  2,  3],
         [ 4,  5,  6,  7],
         [ 8,  9, 10, 11],
```

```
        [12, 13, 14, 15]]),
 tensor([12, 13, 14, 15]),
 tensor([[ 4,  5,  6,  7],
        [ 8,  9, 10, 11]]))
```

- Can also index using binary tensor

[34]:
```
A = torch.arange(0, 12, 1).reshape((3, 4))
B = 5 * torch.ones((3, 4))
A, B, A[A > B]
```

[34]:
```
(tensor([[ 0,  1,  2,  3],
         [ 4,  5,  6,  7],
         [ 8,  9, 10, 11]]),
 tensor([[5., 5., 5., 5.],
         [5., 5., 5., 5.],
         [5., 5., 5., 5.]]),
 tensor([ 6,  7,  8,  9, 10, 11]))
```

2.2 Automatic Calculation of Gradients

- In practice, based on our designed model, the system builds a **computational graph**, tracking which data combined through which operations to produce the output. Automatic differentiation enables the system to subsequently **backpropagate gradients**.
  - Here *backpropagate* simply means to trace through the computational graph, filling in the partial derivatives with respect to each parameter

2.2.1 Intuition

- All computation can be broken into simple components
  - sum
  - multiply
  - exponential
  - convolution
  - ...
- Derivatives for each simple component can be derived mathematically
- Derivatives for **any composition** can be derived via **chain rule**

2.2.2 Forward Mode Mathematical Representation via a simple example

- For a function

$$f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$

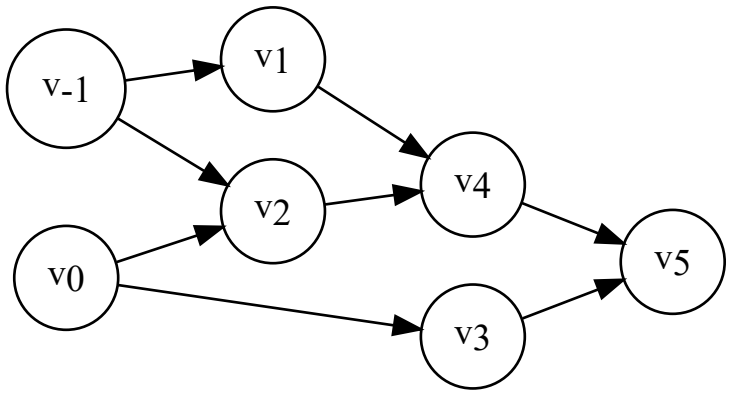
the forward mode computation graph is shown below

[35]:
```
from graphviz import Digraph

f = Digraph('ComputationGraph')
f.attr(rankdir='LR')
f.attr('node', shape='circle')
```

```
f.node('v_-1', label='<v<sub>-1</sub>>')
f.node('v_0', label='<v<sub>0</sub>>')
f.node('v_1', label='<v<sub>1</sub>>')
f.node('v_2', label='<v<sub>2</sub>>')
f.node('v_3', label='<v<sub>3</sub>>')
f.node('v_4', label='<v<sub>4</sub>>')
f.node('v_5', label='<v<sub>5</sub>>')
f.edge('v_-1', 'v_1')
f.edge('v_-1', 'v_2')
f.edge('v_0', 'v_2')
f.edge('v_0', 'v_3')
f.edge('v_1', 'v_4')
f.edge('v_2', 'v_4')
f.edge('v_4', 'v_5')
f.edge('v_3', 'v_5')
f
```

[35]:



- To find the **partial derivate** $\frac{\partial f}{\partial x_1}$ when $x_1 = 2, x_2 = 5$, the Forward Evaluation Trace and Derivative Trace is:
  1. Give the initial value and set initial derivative, notice the derivative of x_1 is set to be one while derivative of x_2 is set to 0

$$v_{-1} = x_1 = 2 \quad v_0 = x_2 = 5$$
$$\dot{v}_{-1} = \dot{x}_1 = 1^{,} \quad \dot{v}_0 = \dot{x}_2 = 0$$

  2. Calculate v_1 and v_2 while keep tracking their derivatives

$$v_1 = \ln v_{-1} = \ln 2 \qquad v_2 = v_{-1} \times v_0 = 10$$
$$\dot{v}_1 = \dot{v}_{-1}/v_{-1} = 1/2^{,} \quad \dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1} = 1 \times 5 + 0 \times 2$$

  3. Calculate v_3 and v_4 while keep tracking their derivatives

$$v_3 = \sin v_0 = \sin 5 \qquad v_4 = v_1 + v_2 = 0.693 + 10$$
$$\dot{v}_3 = \dot{v}_0 \times \cos v_0 = 0 \times \cos 5^{,} \quad \dot{x}_4 = \dot{v}_1 + \dot{v}_2 = 0.5 + 5$$

4. Get the final result and derivative

$$y = v_5 = v_4 - v_3 = 10.693 + 0.959$$
$$\dot{y} = \dot{v}_5 = \dot{v}_4 - \dot{v}_3 = 5.5 - 0$$

5. Therefore, the result is

$$\frac{\partial f}{\partial x_1} = 5.5|_{x_1=2,x_2=5}$$

- Therefore, for a n-dimensional input and 1-dimensional output
  - Only calculate once for the output
  - Need to calculate n times for all the partial derivatives.
    - Each time set one initial derivative to be 1 and other initial derivative to be 0
  - **Low efficiency** when n is large, which is common in complex models

2.2.3 Build the computation graph by tracking data

- PyTorch automatically creates a computation graph if **requires_grad=True**
- For a given variable with **requires_grad=True**, identify the operations

[ ]: