Autograd, optimizare

Bibliografie:

1. Deep Learning with PyTorch, Eli Stevens, Luca Antiga, Thomas Viehmann, Manning; 1st edition (August 4, 2020)
2. PyTorch Pocket Reference: Building and Deploying Deep Learning Models, by Joe Papa, O'Reilly Media; 1st edition (June 1, 2021)

In [1]:
```
import torch
print(f'Versiune torch: {torch.__version__}')
```

```
Versiune torch: 2.0.0+cu118
```

In [2]:
```
torch.cuda.is_available()
```

Out[2]:
```
True
```

Calcul de gradienti cu autograd

Calculul derivatelor partiale ale unei functii este crucial pentru algoritmii actuali de machine learning. Modificand ponderile (parametrii, coeficientii) unei functii, se poate face printr-un proces iterativ aducerea functiei intr-o zona in care gradientii sa fie 0.

Exemplul 1: functie de o singura variabila

In [3]:
```
# definim o variabila x. Pentru ca se va calcula derivata unei funcii in raport cu x,
# faptul ca trebuie considerat x pentru calcul de gradient
x = torch.tensor(10.0, requires_grad = True)
print(x)
# x trebuie dat ca valoare floating point;
# o valoare initiala data ca intreg (10) face ca tensorul sa aiba datatype intreg.
# In PyTorch gradientii se pot calcula numai pentru cantitati floating point
```

```
tensor(10., requires_grad=True)
```

Verificam daca tensorul x are gradient definit in acest moment:

In [4]:
```
x.grad is None
```

Out[4]:
```
True
```

Definim o expresie care depinde de x, de exemplu $$ y = 5x^3 -x^2 + 2*x -100 $$ Derivata lui y in functie de x este $$ \frac{dy}{dx} = 15x^2-2x+2 $$ care evaluata pentru $x = 10$ da rezultatul 1482.

In [5]:
```
y = 5*x**3 - x ** 2 + 2*x - 100
# declansam calculul de gradient. Metoda backward() poate fi chemata pentru un tensor
```

```
y.backward()
```

Din acest moment, tensorul x are gradient, calculat de metoda `backward`:

In [6]:
```
# verificam daca s-a calculat un gradient pentru x, corespunzator lui dy/dx:
print(f'Avem gradient pe x: {x.grad is not None}')
```

```
Avem gradient pe x: True
```

In [7]:
```
# recuperam gradientul:
dydx = x.grad
dydx
```

Out[7]:
```
tensor(1482.)
```

Important! Daca mai apelam odata backward() pe o expresie care il foloseste pe x (de exemplu: aceeasi expresie y ca mai sus), atunci se calculeaza din nou gradient pentru vectorul x si se acumuleaza la cel calculat deja. Ca atare, pentru acelasi y noul gradient este 1482 + 1482 = 2964:

In [8]:
```
y = 5*x**3 - x ** 2 + 2*x - 100
y.backward()
x.grad
```

Out[8]:
```
tensor(2964.)
```

Exemplul 2: functie de 2 variabile

Consideram functia: $$ z(x, y) = x^2 + y^5 - x^2\cdot y $$ Derivatele partiale sunt: $$ \frac{\partial z}{\partial x} = 2x-2xy $$ respectiv $$ \frac{\partial z}{\partial y} = 5y^4-x^2 $$

Pentru $x=3, y=4$ cele doua derivate partiale au valorile: $$ \frac{\partial z}{\partial x} = -18 $$ si respectiv $$ \frac{\partial z}{\partial y} = 1271 $$

In [9]:
```
x=torch.tensor(3.0, requires_grad=True)
y=torch.tensor(4.0, requires_grad=True)
z=x**2+y**5-x**2*y
z.backward()
```

In [10]:
```
# recuparam gradientii dz/dx, dz/dy
print(f'gradient dupa x={x.grad}\ngradient dupa y={y.grad}')
```

```
gradient dupa x=-18.0
gradient dupa y=1271.0
```

Exemplul 3: functie de eroare patratica, mai multe ponderi instruibile

In PyTorch se pot calculaautomat gradientii chiar daca sunt folositi in interiorul unor functii definite de utilizator.

In [11]:
```
def f(w: torch.Tensor, x: torch.Tensor) -> torch.Tensor:
    return x.dot(w)

def error_function(y: torch.Tensor, y_hat: torch.Tensor) -> torch.Tensor:
    return (y - y_hat) ** 2

# x: valori de intrare
x = torch.tensor([1.0, 4.0, -3.0, 5.0, 4.0])
print(f'Verificam daca tensorul x e pregatit sa aiba gradient calculat: {x.requires_gr
# w: ponderi
w = torch.rand_like(x, requires_grad=True)

ground_truth = 10

# eroare patratica medie
error = error_function(ground_truth, f(w, x))
print(f'Eroare de predictie: error={error}')

# se calculeaza gradientii de catre Pytorch
error.backward()
print(f'Gradientii pentru w: {w.grad}')

print(f'Gradientii pentru x nu se calculeaza, deoarece tensorul x are requires_grad=Fa
print(f'\tx.grad is None={x.grad is None}')
```

```
Verificam daca tensorul x e pregatit sa aiba gradient calculat: False
Eroare de predictie: error=23.257722854614258
Gradientii pentru w: tensor([ -9.6453, -38.5810,  28.9358, -48.2263, -38.5810])
Gradientii pentru x nu se calculeaza, deoarece tensorul x are requires_grad=False
        x.grad is None=True
```

In [12]:
```
# aplicam un gradient descent manual: din ponderile actuale se scade gradientul
# inmultit cu un learning rate mic
lr = 0.01
w = w - lr * w.grad
error = error_function(ground_truth, f(w, x))
print(f'Noua eroare: {error}')
# se constata scaderea erorii
```

```
Noua eroare: 2.6885907649993896
```

Optimizare manuala

In [13]:
```
# model de predictie
def model(x, w, b):
    return w * x + b

# functia de cost
def error(y_hat: torch.Tensor, y: torch.Tensor, weights: torch.Tensor, lmbda: float) -
    quality_error = torch.mean((y_hat - y)**2)
    regularization = lmbda * weights.norm() ** 2
    return quality_error + regularization
```

In [15]:
```
import matplotlib.pyplot as plt

params = torch.tensor([1.0, 0.0], requires_grad=True)
x = torch.tensor(20.0)
```

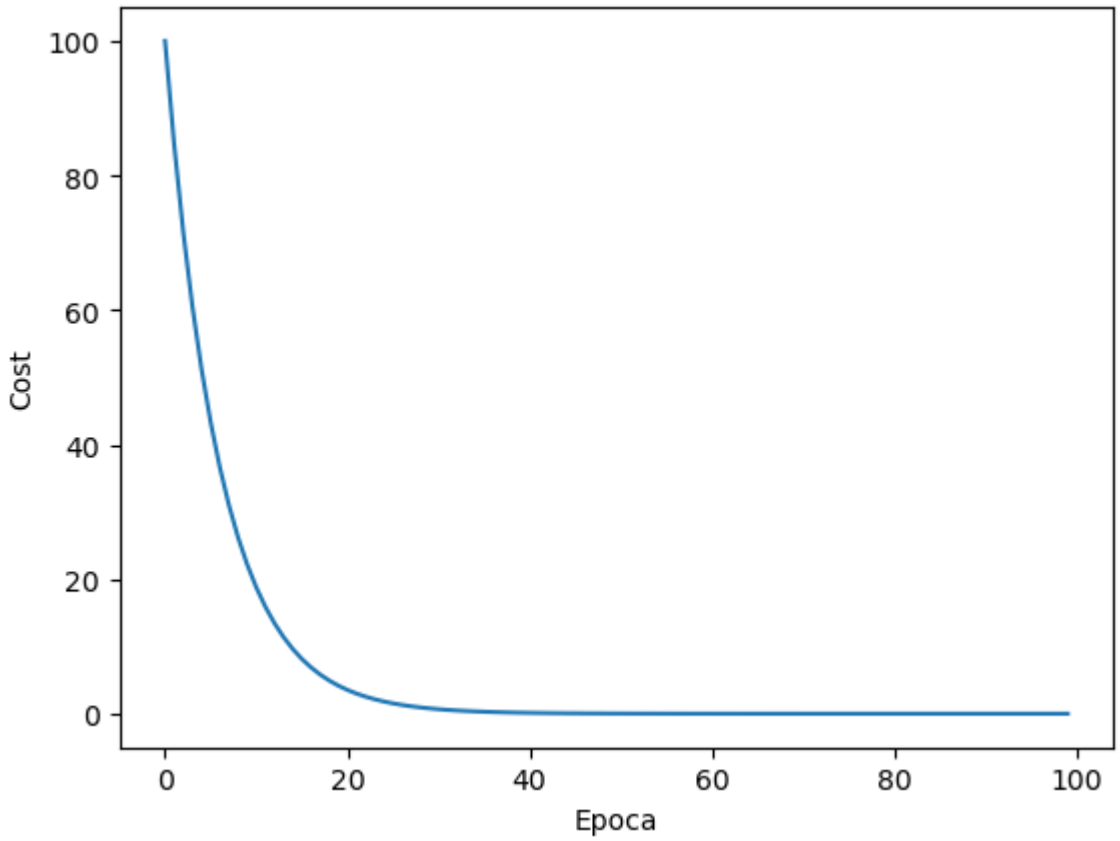
```
# la inceput, gradientii pt ponderi nu sunt calculati
print(f'params.grad is None: {params.grad is None}')

y_true = torch.tensor(10)
learning_rate = 0.0001
n_iters = 100
lmbda = 1.0

losses = []

for i in range(1, n_iters+1):
    # gradientii calculati in mod repetat se acumuleaza (insumeaza cu gradientii calcu
    # evitam aceasta insumare prin setarea lor explicita la 0
    if params.grad is not None:
        params.grad.zero_()

    y_hat = model(x, *params)
    loss = error(y_hat, y_true, params[1:], lmbda)
    losses.append(loss.detach().item())
    if i % 10 == 0:
        print(f'Iteration: {i}, loss: {loss}')
    loss.backward()

    with torch.no_grad():
        assert params.grad is not None
        params -= learning_rate * params.grad
```

```
params.grad is None: True
Iteration: 10, loss: 22.206819534301758
Iteration: 20, loss: 4.172554969787598
Iteration: 30, loss: 0.7844100594520569
Iteration: 40, loss: 0.1478678286075592
Iteration: 50, loss: 0.028277603909373283
Iteration: 60, loss: 0.005807911511510611
Iteration: 70, loss: 0.001584485056810081
Iteration: 80, loss: 0.0007890488486737013
Iteration: 90, loss: 0.0006376549135893583
Iteration: 100, loss: 0.0006072467076592147
```

Nota: daca celula de plot produce eroare, atunci se foloseste workaround de la https://stackoverflow.com/questions/53014306/error-15-initializing-libiomp5-dylib-but-found-libiomp5-dylib-already-initial:

In [16]:
```
import os
os.environ["KMP_DUPLICATE_LIB_OK"]="TRUE"
```

In [17]:
```
plt.plot(losses)
plt.xlabel('Epoca')
plt.ylabel('Cost')
plt.show()
```



Optimizatori Pytorch

Mai sus s-a implementat in mod manual algoritmul de SGD, doar pentru a demonstra calculul gradientilor si efectul asupra ponderilor. De regula, se foloseste un agloritm de optimizare predefinit care aplica gradientii pe ponderi. O lista a optimizatorilor implementati in Pytorch este data mai jos.

In [18]:
```
import torch.optim as optim
[opt for opt in dir(optim) if opt[0].isupper()]
```

Out[18]:
```
['ASGD',
 'Adadelta',
 'Adagrad',
 'Adam',
 'AdamW',
 'Adamax',
 'LBFGS',
 'NAdam',
 'Optimizer',
 'RAdam',
 'RMSprop',
 'Rprop',
 'SGD',
 'SparseAdam']
```

Fiecare optimizator preia o lista de parametri (de ex ponderile unui model de predictie). Dupa ce gradientii pentru minibatchul curent sunt calculati, se aplica in mod corespunzator pe ponderi.

In [19]:
```
x = torch.tensor(20.0)
params = torch.tensor([1.0, 0.0], requires_grad=True)
learning_rate = 1e-3
optimizer = optim.SGD([params], lr=learning_rate)
```

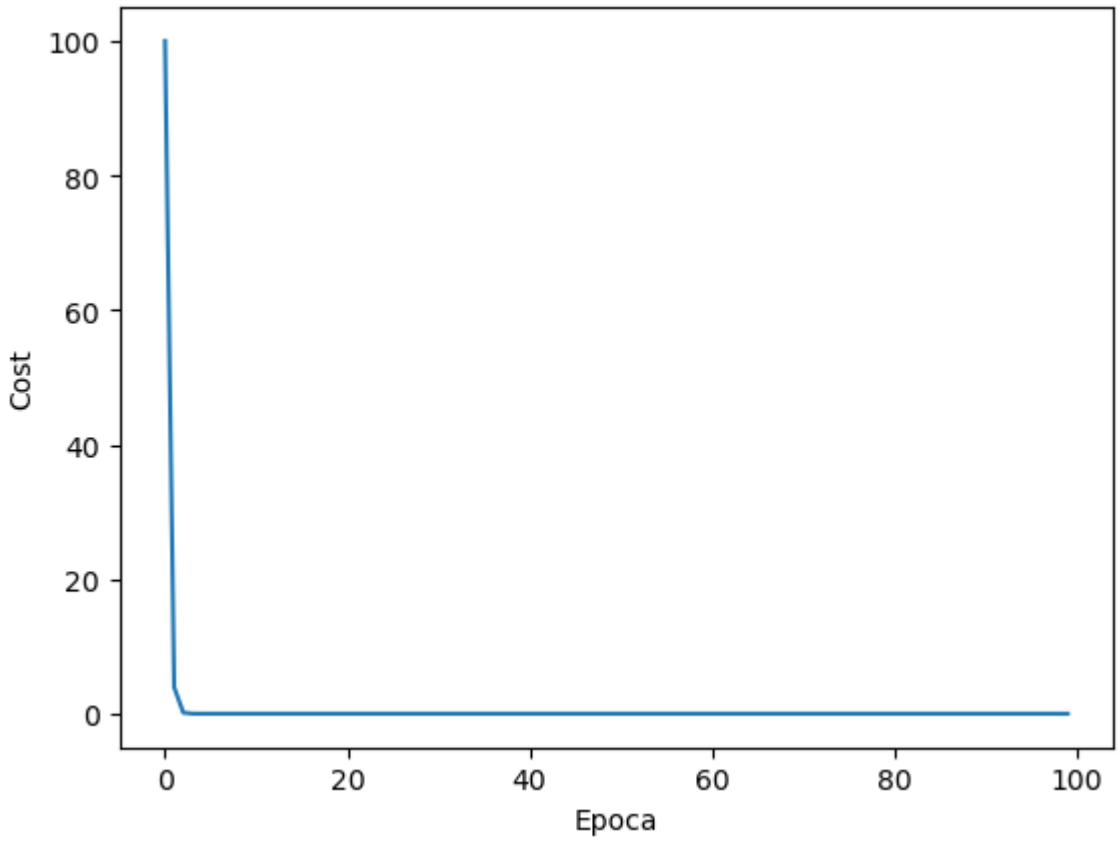
Secventa care urmeaza are acelasi scop ca si ciclarea din sectiunea anterioara: se modifica ponderile pentru a face minimizarea functiei `error`.

In [20]:
```
losses = []

for epoch in range(1, n_iters + 1):
    y_hat = model(x, *params)
    loss = error(y_hat, y_true, params[1:],  lmbda)
    losses.append(loss.item())
    print(f'Iteration: {epoch}, loss: {loss}')
    # se pun gradientii anterior calculati pe 0. Intrucat optimizatorul este responsab
    # managementul ponderilor, resetarea gradientilor este facuta prin intermediul lui
    optimizer.zero_grad()

    # calcul de derivate partiale
    loss.backward()

    # se modifica ponderile folosind gradientii calculati de apelul backward()
    optimizer.step()
```

```
Iteration: 1, loss: 100.0
Iteration: 2, loss: 3.9207983016967773
Iteration: 3, loss: 0.15429987013339996
Iteration: 4, loss: 0.006642207968980074
Iteration: 5, loss: 0.0008512443164363503
Iteration: 6, loss: 0.000621881103143096
Iteration: 7, loss: 0.0006105515058152378
Iteration: 8, loss: 0.000607771216891706
Iteration: 9, loss: 0.0006053348770365119
Iteration: 10, loss: 0.0006029214127920568
Iteration: 11, loss: 0.0006005181348882616
Iteration: 12, loss: 0.000598124461248517
Iteration: 13, loss: 0.0005957404500804842
Iteration: 14, loss: 0.0005933656939305365
Iteration: 15, loss: 0.0005910006002523005
Iteration: 16, loss: 0.0005886448197998106
Iteration: 17, loss: 0.0005862982361577451
Iteration: 18, loss: 0.0005839611985720694
Iteration: 19, loss: 0.0005816334742121398
Iteration: 20, loss: 0.0005793151794932783
Iteration: 21, loss: 0.0005770060233771801
Iteration: 22, loss: 0.0005747061804868281
Iteration: 23, loss: 0.0005724154179915786
Iteration: 24, loss: 0.0005701337940990925
Iteration: 25, loss: 0.0005678612506017089
Iteration: 26, loss: 0.0005655977874994278
Iteration: 27, loss: 0.0005633432883769274
Iteration: 28, loss: 0.0005610977532342076
Iteration: 29, loss: 0.0005588610656559467
Iteration: 30, loss: 0.0005566334584727883
Iteration: 31, loss: 0.0005544146406464279
Iteration: 32, loss: 0.0005522047867998481
Iteration: 33, loss: 0.0005500036641024053
Iteration: 34, loss: 0.0005478113889694214
Iteration: 35, loss: 0.0005456277285702527
Iteration: 36, loss: 0.0005434528575278819
Iteration: 37, loss: 0.0005412864848040044
Iteration: 38, loss: 0.0005391290178522468
Iteration: 39, loss: 0.0005369800492189825
Iteration: 40, loss: 0.0005348395206965506
Iteration: 41, loss: 0.0005327076651155949
Iteration: 42, loss: 0.0005305844824761152
Iteration: 43, loss: 0.0005284695071168244
Iteration: 44, loss: 0.0005263631464913487
Iteration: 45, loss: 0.0005242649931460619
Iteration: 46, loss: 0.0005221752799116075
Iteration: 47, loss: 0.0005200940067879856
Iteration: 48, loss: 0.0005180207663215697
Iteration: 49, loss: 0.0005159559659659863
Iteration: 50, loss: 0.0005138994310982525
Iteration: 51, loss: 0.0005118509288877249
Iteration: 52, loss: 0.000509810633957386
Iteration: 53, loss: 0.0005077786045148969
Iteration: 54, loss: 0.0005057546077296138
Iteration: 55, loss: 0.0005037385853938758
Iteration: 56, loss: 0.0005017306539230049
Iteration: 57, loss: 0.00049973075510934
Iteration: 58, loss: 0.0004977386561222374
Iteration: 59, loss: 0.0004957547062076628
Iteration: 60, loss: 0.0004937786725349724
```

```
Iteration: 61, loss: 0.0004918103804811835
Iteration: 62, loss: 0.0004898500046692789
Iteration: 63, loss: 0.0004878975742030889
Iteration: 64, loss: 0.0004859527107328176 5
Iteration: 65, loss: 0.0004840158799197525
Iteration: 66, loss: 0.0004820864996872842 3
Iteration: 67, loss: 0.0004801649774890393
Iteration: 68, loss: 0.0004782510804943740 4
Iteration: 69, loss: 0.0004763447504956275
Iteration: 70, loss: 0.0004744461621157825
Iteration: 71, loss: 0.0004725549661088735
Iteration: 72, loss: 0.0004706713370978832
Iteration: 73, loss: 0.0004687953914981335 4
Iteration: 74, loss: 0.0004669267800636589 5
Iteration: 75, loss: 0.0004650656774174422
Iteration: 76, loss: 0.0004632119671441614 6
Iteration: 77, loss: 0.0004613656783476472
Iteration: 78, loss: 0.000459526723716408
Iteration: 79, loss: 0.0004576951032504439 4
Iteration: 80, loss: 0.0004558708169497549 5
Iteration: 81, loss: 0.0004540536901913583 3
Iteration: 82, loss: 0.0004522438684944063 4
Iteration: 83, loss: 0.0004504412354435771 7
Iteration: 84, loss: 0.0004486457619350403 5
Iteration: 85, loss: 0.000446857389761135
Iteration: 86, loss: 0.0004450763226486742 5
Iteration: 87, loss: 0.0004433022113516927
Iteration: 88, loss: 0.0004415352887008339
Iteration: 89, loss: 0.0004397755292761623 86
Iteration: 90, loss: 0.0004380222235340625
Iteration: 91, loss: 0.0004362761974334717
Iteration: 92, loss: 0.0004345371562521904 7
Iteration: 93, loss: 0.0004328051873017102 5
Iteration: 94, loss: 0.0004310799413360655 3
Iteration: 95, loss: 0.0004293615347705781 5
Iteration: 96, loss: 0.000427650171332061 3
Iteration: 97, loss: 0.0004259455308783799 4
Iteration: 98, loss: 0.0004242424761340953 41
Iteration: 99, loss: 0.0004225565644446760 4
Iteration: 100, loss: 0.0004208721511531621
```

In [21]:
```
plt.plot(losses)
plt.xlabel('Epoca')
plt.ylabel('Cost')
plt.show()
```



In [ ]: