CodeLabs – Optimization

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2023

Program

1. Gradients and Automatic Differerntiation

2. Unconstrained optimization

3. Constrained optimization

4. Stochastic gradient

BASICS

Why optimize?

- All the problems that we address in this course entail optimization:

  $\Rightarrow$ Inverse problems
  - $\rightarrow$ data assimilation problems
  - $\rightarrow$ parameter identification problems

  $\Rightarrow$ Surrogate modelling

  $\Rightarrow$ Machine Learning

- They are all based on the underlying theoretical problem:

  $\Rightarrow$ minimize a cost/objective/loss function over a vector- or function-space of coefficients

UNCONSTRAINED OPTIMIZATION

Numpy

- Comparison of gradient descent and stochastic gradient

  $\Rightarrow$ `02Examples/opt/GDvsSGD.ipynb`

- Comparison of different algorithms on a non-convex, 2D problem

  $\Rightarrow$ `02Examples/opt/opt_himmelblau.ipynb`

- Comparison of different initial guesses for a non-convex, 2D problem, with animation

  $\Rightarrow$ `02Examples/opt/opt_visu.ipynb`

PyTorch

- PyTorch for 1D optimization problems

  ⇒ (02Examples/opt/torch-opt-simplest.ipynb)

- Pytorch detailed comparison and diagnostics of SGD and LBFGS methods

  ⇒ (02Examples/opt/torch_lbfgs_convergence.ipynb)

- Pytorch linear regression curve fitting by least-squares minimization

  ⇒ 02Examples/opt/torch_linreg_basic.ipynb

- Pytorch exponential curve fitting by least-squares minimization using Adam

  ⇒ 02Examples/opt/torch_curve_fitting.ipynb

CONSTRAINED OPTIMIZATION

Scipy - minimize

- Quadratic function with equality constraint using Scipy's 'minimize' function

  $\Rightarrow$ `02Examples/opt/Constrained_opt.ipynb`

- Quadratic function with inequality constraint using Scipy's 'minimize' function

  $\Rightarrow$ `02Examples/opt/Constrained_inequality.ipynb`

AUTOMATIC DIFFERENTIATION

Autograd

- Introduction to differentiable programming

  $\Rightarrow$ 02Examples/ad/diff_prog.ipynb

- Simple linear regression with 'autograd'

  $\Rightarrow$ 02Examples/ad/autograd_lin_reg.ipynb

- 'autograd' tutorial

  $\Rightarrow$ 02Examples/ad/autograd_tut.ipynb

References

1. Please consult the list provided on the website:
   CODE REFERENCES