Week 7 February 14-18: Finalization of importance sampling, start Gradient methods, steepest descent and Conjugate Gradient Methods

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Overview of week 7, February 14-18

Topics.

- Finalize discussion on importance sampling and Fokker-Planck and Langevin equations

- Gradient Descent methods, Steepest Descent

- Conjugate Gradient Descent

Teaching Material, videos and written material.

- On importance sampling, see notes from last week at `http://compphysics.github.io/ComputationalPhysics2/doc/pub/week4/html/week4-reveal.html`

- These lecture notes

- Recommended background literature, Convex Optimization by Boyd and Vandenberghe. Their lecture slides are very useful (warning, these are some 300 pages).

Motivation

Our aim with this part of the project is to be able to

- find an optimal value for the variational parameters using only some few Monte Carlo cycles

- use these optimal values for the variational parameters to perform a large-scale Monte Carlo calculation

To achieve this will look at methods like *Steepest descent* and the *conjugate gradient method.* Both these methods allow us to find the minima of a multi-variable function like our energy (function of several variational parameters). Alternatively, you can always use Newton's method. In particular, since we will normally have one variational parameter, Newton's method can be easily used in finding the minimum of the local energy.

Simple example and demonstration

Let us illustrate what is needed in our calculations using a simple example, the harmonic oscillator in one dimension. For the harmonic oscillator in one-dimension we have a trial wave function and probability

$$\psi_T(x;\alpha) = \exp{-(\frac{1}{2}\alpha^2 x^2)},$$

which results in a local energy

$$\frac{1}{2}\left(\alpha^2 + x^2(1 - \alpha^4)\right).$$

We can compare our numerically calculated energies with the exact energy as function of α

$$\overline{E}[\alpha] = \frac{1}{4}\left(\alpha^2 + \frac{1}{\alpha^2}\right).$$

Simple example and demonstration

The derivative of the energy with respect to α gives

$$\frac{d\langle E_L[\alpha]\rangle}{d\alpha} = \frac{1}{2}\alpha - \frac{1}{2\alpha^3}$$

and a second derivative which is always positive (meaning that we find a minimum)

$$\frac{d^2\langle E_L[\alpha]\rangle}{d\alpha^2} = \frac{1}{2} + \frac{3}{2\alpha^4}$$

The condition

$$\frac{d\langle E_L[\alpha]\rangle}{d\alpha} = 0,$$

gives the optimal $\alpha = 1$, as expected.

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Exercise 1: Find the local energy for the harmonic oscillator
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a) Derive the local energy for the harmonic oscillator in one dimension and find its expectation value.
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b) Show also that the optimal value of optimal $\alpha = 1$
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c) Repeat the above steps in two dimensions for N bosons or electrons. What is the optimal value of α?

Variance in the simple model

We can also minimize the variance. In our simple model the variance is

$$\sigma^2[\alpha] = \frac{1}{4}\left(1 + (1-\alpha^4)^2 \frac{3}{4\alpha^4}\right) - \overline{E}^2.$$

which yields a second derivative which is always positive.

Computing the derivatives

In general we end up computing the expectation value of the energy in terms of some parameters $\alpha_0, \alpha_1, \ldots, \alpha_n$ and we search for a minimum in this multi-variable parameter space. This leads to an energy minimization problem *where we need the derivative of the energy as a function of the variational parameters.*

In the above example this was easy and we were able to find the expression for the derivative by simple derivations. However, in our actual calculations the energy is represented by a multi-dimensional integral with several variational parameters. How can we can then obtain the derivatives of the energy with respect to the variational parameters without having to resort to expensive numerical derivations?

Expressions for finding the derivatives of the local energy

To find the derivatives of the local energy expectation value as function of the variational parameters, we can use the chain rule and the hermiticity of the Hamiltonian.

Let us define

$$\bar{E}_\alpha = \frac{d\langle E_L[\alpha]\rangle}{d\alpha}.$$

as the derivative of the energy with respect to the variational parameter α (we limit ourselves to one parameter only). In the above example this was easy and

we obtain a simple expression for the derivative. We define also the derivative of the trial function (skipping the subindex T) as

$$\bar{\psi}_\alpha = \frac{d\psi[\alpha]\rangle}{d\alpha}.$$

Derivatives of the local energy

The elements of the gradient of the local energy are then (using the chain rule and the hermiticity of the Hamiltonian)

$$\bar{E}_\alpha = 2\left(\langle\frac{\bar{\psi}_\alpha}{\psi[\alpha]}E_L[\alpha]\rangle - \langle\frac{\bar{\psi}_\alpha}{\psi[\alpha]}\rangle\langle E_L[\alpha]\rangle\right).$$

From a computational point of view it means that you need to compute the expectation values of

$$\langle\frac{\bar{\psi}_\alpha}{\psi[\alpha]}E_L[\alpha]\rangle,$$

and

$$\langle\frac{\bar{\psi}_\alpha}{\psi[\alpha]}\rangle\langle E_L[\alpha]\rangle$$

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Exercise 2: General expression for the derivative of the energy
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a) Show that

$$\bar{E}_\alpha = 2\left(\langle\frac{\bar{\psi}_\alpha}{\psi[\alpha]}E_L[\alpha]\rangle - \langle\frac{\bar{\psi}_\alpha}{\psi[\alpha]}\rangle\langle E_L[\alpha]\rangle\right).$$

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b) Find the corresponding expression for the variance.