Metropolis

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Introduzione

Obiettivi

- E' il Machine Learning applicabile per calcolare l'energia di ground state di un Condensato di Bose-Einstein (BEC)?
- Possiamo imparare qualcosa in più sulla Restricted Boltzmann Machine?

Ingredienti base

1. Metodi Variational Monte Carlo per calcolare l'energia
2. Funzione d'onda di prova rappresentata con Restricted Boltzmann Machine
3. Parametri variazionali modificati con Stochastic Gradient Descent

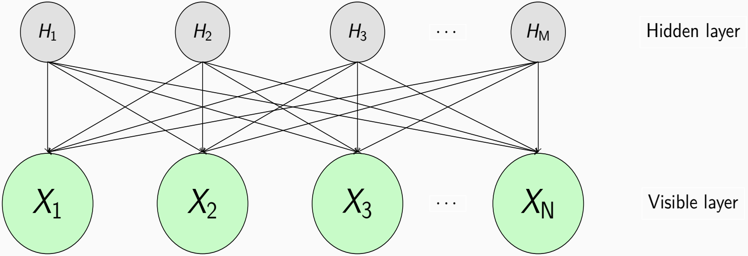
Machine Learning

- Set of algorithms to give computers the ability to learn to recognize images (e.g. plants, handwritten numbers) or data distribution
- Huge success in the last years: Google Translate, ...
- Recent applications in physics with many-body problems such as Ising Model and Heisenberg model[1], with encouraging results

[1] Giuseppe Carleo and Matthias Troyer. "Solving the quantum many-body problem with artificial neural networks". In: *Science* 355.6325 (2017), pp. 602–606. ISSN: 0036-8075. DOI: 10.1126/science.aag2302. eprint: http://science.sciencemag.org/content/355/6325/602.full.pdf. URL: http://science.sciencemag.org/content/355/6325/602.

Machine Learning

We represent our trial wave-function with a set of artificial Neural Networks. We call this way of representing the trail wave-function, Neural-Network Quantum State (NQS). The architecture selected is the Restricted Boltzmann Machine. The goal of the RBM is to learn the probability distribution of the simulated system. In quantum systems the probability distribution is the wave-function Ψ.



The joint probability distribution of the RBM is defined as

$$F_{RBM}(\mathbf{X}, \mathbf{H}) = \frac{1}{Z} \exp(-E(\mathbf{X}, \mathbf{H})),$$

where $\mathbf{X}$ is the visible nodes and $\mathbf{H}$ is the hidden nodes. The quantity Z represents the partition function or normalization constant of the system.

The quantity $E(\mathbf{X}, \mathbf{H})$ is the function that specifies the relation between the visible and hidden nodes. It is called the energy of the node configuration. The choice of $E(\mathbf{X}, \mathbf{H})$ is the heart of what sort of RBM we have.

Machine Learning

There are several types of RBM. Since, in our case, the visible nodes need to take continuous values, we choose the Gaussian-Binary RBM:

$$E(\mathbf{X}, \mathbf{H}) = \sum_{i}^{\mathrm{N}} \frac{(X_i - a_i)^2}{2\sigma} - \sum_{j}^{\mathrm{M}} b_j H_j + \sum_{ij}^{\mathrm{N,M}} \frac{X_i w_{ij} H_j}{\sigma^2},$$

To represent the wave-function, we use the so-called "marginal PDF" found by summing over all the hidden nodes:

$$\Psi(\mathbf{X}) = \sum_{H} F_{RBM}(\mathbf{X}, \mathbf{H}) = \frac{1}{Z} \sum_{H} \exp(-E(\mathbf{X}, \mathbf{H})).$$

Setting in the Gaussian-Binary RBM gives the final result

$$\Psi(\mathbf{X}) = \frac{1}{Z} \exp\left[-\sum_{i}^{\mathrm{N}} \frac{(X_i - a_i)^2}{2\sigma^2} \right] \prod_{j}^{\mathrm{M}} \left(1 + \exp\left[b_j + \sum_{i}^{\mathrm{N}} \frac{X_i w_{ij}}{\sigma^2} \right] \right).$$

Condensato di Bose-Einstein

- Stato della materia in cui gas diluiti di bosoni vengono sottoposti a una transizione di fase quando vengono raffreddati fino a basse temperature ($T \to 0$ K). La maggior parte dei bosoni condensa nel ground state. Questo causa nuovi fenomeni quantistici come superfluidità e coerenza di fase.
- Predetto da A. Einstein nel 1925 seguendo il lavoro del fisico indiano S. N. Bose (1924) sulla statistica dei bosoni.
- Verificati sperimentalmente nel 1995 dal team di Cornell e Wieman a Boulder con ^{87}Rb e da Ketterle al MIT con ^{23}Na raffreddati a temperature di 100 nK attraverso laser cooling e evaporative cooling in trappole magneto-ottiche. Premio Nobel 2001.

Gross-Pitaevskii equation

Negli esperimenti sono stati utilizzati gas diluiti (e.g. atomi alcalini) e non uniformi perchè confinati in trappole magneto-ottiche. L'equazione di riferimento è l'equazione di Gross-Pitaevskii (GP):

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2\right)\Psi(\mathbf{r},t)$$

dove $i = \sqrt{-1}, \hbar$ è la costante di Planck ridotta, t è il tempi, Ψ è la funzione d'onda del condensato, $\mathbf{r}$ rappresenta la posizione dei bosoni e V è il potenziale esterno che intrappola i bosoni. La quantità g è la costante di accoppiamento

$$g = \frac{4\pi\hbar^2 a}{m}$$

dove a is la lunghezza di scattering dell'onda s. Confronteremo le sue soluzioni in [2] con i nostri risultati.

Motivazioni

La condizione di diluizione è data dal parametro na^3, dove n è la densità del sistema. Quando il parametro è piccolo, GP funziona molto bene. Tuttavia ci sono esperimenti in cui il parametro supera tale valore. A qual punto è importante studiare il sistema con un approccio many-body. In letterature, troviamo molti papers in cui vengono utilizzati metodi Monte Carlo nel range diluito fino alla densità dell'^{4}He. Per esempio:

1. in [3], Dubois e Glyde usano Variational Monte Carlo (VMC);
2. in [4], Giorgini et al. usano Diffusion Monte Carlo (DMC);
3. in [5], Grüter et al. usano the path-integral Monte Carlo.

In this thesis, we use ML and we compare the results with GP equation since we consider a diluite system. Nevertheless, out of the diluite range, we note that ML results should be compared to the Monte Carlo ones which we have briefly mentioned above.

Metodi

Il sistema

We consider a gas of N_p bosons in spherical and elliptical harmonic oscillator potentials. The interaction between bosons in modeled by the hard-core model as in [3]. The Hamiltonian of the system is

$$H = \sum_{i=1}^{N_p} \left[-\frac{1}{2} \frac{\hbar^2}{m} \nabla_i^2 + V_{ext}(\mathbf{r}_i) \right] + \sum_{i \neq k} V_{int}(r_{ik}), \tag{1}$$

where $V_{ext}(\mathbf{r})$ is the harmonic oscillator potential given by

$$V_{ext}(\mathbf{r}) = \begin{cases} \frac{1}{2} m \omega_{ho}^2 r^2 & \text{Spherical} \\ \frac{1}{2} m \left[\omega_{ho}^2 \left(x^2 + y^2 \right) + \omega_z^2 z^2 \right] & \text{Elliptical} \end{cases}$$

and $V_{int}(r_{ik})$ is the hard-shell interaction potential

$$V_{int}(r_{ik}) = \begin{cases} 0, & r_{ik} > a \\ \infty, & r_{ik} < a. \end{cases}$$

The quantity $r_{ik} = |\mathbf{r}_i - \mathbf{r}_k|$ represents the distance between particle i and k, while a is the size of the interaction between particles.

No interaction - spherical trap

When we set the interaction to be zero ($V_{int} = 0$), we are left with a harmonic oscillator potential, where we consider a spherical shape for simplicity. In this case the solutions are known analytically. In general the energy is given by $E_n = \hbar\omega_{ho}(n + \frac{1}{2})$. The ground state is

$$E(N_p, D) = \frac{1}{2}\mathrm{D}N_p\ \hbar\omega_{ho}.$$

where D is the dimension of the system and N_p is the number of particles. This case is useful to benchmark our code at the beginning.

No interaction - elliptic trap

The interaction is still null ($V_{int} = 0$), the trap now is considered to be elliptic.
Let us introduce lengths in unit of $a_{ho} = \sqrt{\hbar/(m\omega_{ho})}$, $r \to r/a_{ho}$ and energy in units of $\hbar\omega_{ho}$. The Hamiltonian can be rearranged as

$$H = \sum_{k=1}^{N_p} \frac{\hbar\omega_{ho}}{2}\left(- a_{ho}\nabla_k^2 + a_{ho}\hbar\left[x_k^2 + y_k^2 + \frac{\omega_z^2}{\omega_{ho}^2} z_k^2\right]\right).$$

We set $\lambda = \omega_z/\omega_{ho}$, we get

$$H = \sum_{k=1}^{N_p} \frac{1}{2}\left(- \nabla_k^2 + V_{ext}(\mathbf{r}_k)\right) \tag{2}$$

where $V_{ext} = x_k^2 + y_k^2 + \lambda^2 z_k^2$. As in [2], we set $\lambda = \sqrt{8}$. In [3], the energy of non-interacting bosons in this trap is shown to be

$$\frac{E}{N} \to E_{ho} = \hbar\omega_{ho}\left(1 + \frac{\lambda}{2}\right) = 2.414\ \hbar\omega_{ho}.$$

Interaction - elliptic trap

At this point, we turn on the interaction $V_{int} \neq 0$ and we consider an elliptic trap. The Hamiltonian is

$$H = \sum_{k=1}^{N_p} \frac{1}{2}\Big(-\nabla_k^2 + V_{ext}(\mathbf{r}_k)\Big) + \sum_{k<i}^{N_p} V_{int}(\mathbf{r}_k, \mathbf{r}_i). \tag{3}$$

where $V_{ext} = x_k^2 + y_k^2 + \lambda^2 z_k^2$ and $\lambda = \sqrt{8}$ as above.

all small caps

This frame uses the `allsmallcaps` titleformat.

Potential problems

As this titleformat also uses smallcaps you face the same problems as with the `smallcaps` titleformat. Additionally this format can cause some other problems. Please refer to the documentation if you consider using it.

As a rule of thumb: Just use it for plaintext-only titles.

ALL CAPS

This frame uses the `allcaps` titleformat.

Potential Problems

This titleformat is not as problematic as the `allsmallcaps` format, but basically suffers from the same deficiencies. So please have a look at the documentation if you want to use it.

Analisi dati

TYPOGRAPHY

```
The theme provides sensible defaults to
\emph{emphasize} text, \alert{accent} parts
or show \textbf{bold} results.
```

becomes

The theme provides sensible defaults to *emphasize* text, accent parts or show **bold** results.

FONT FEATURE TEST

- Regular
- *Italic*
- SmallCaps
- **Bold**
- ***Bold Italic***
- **Bold SmallCaps**
- `Monospace`
- *`Monospace Italic`*
- **`Monospace Bold`**
- ***`Monospace Bold Italic`***

LISTS

Items

- Milk
- Eggs
- Potatos

Enumerations

1. First,
2. Second and
3. Last.

Descriptions

PowerPoint Meeh.

Beamer Yeeeha.

ANIMATION

- This is important

ANIMATION

- This is important
- Now this

ANIMATION

- This is important
- Now this
- And now this

ANIMATION

- This is really important
- Now this
- And now this

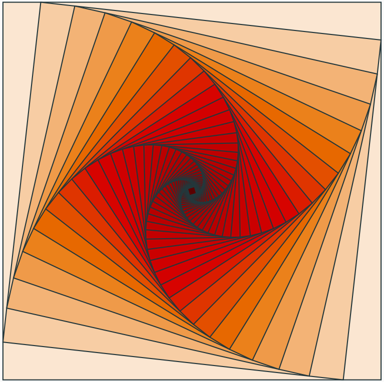


Figure 1: Rotated square from texample.net.

Table 1: Largest cities in the world (source: Wikipedia)

City	Population
Mexico City	20,116,842
Shanghai	19,210,000
Peking	15,796,450
Istanbul	14,160,467

BLOCKS

Three different block environments are pre-defined and may be styled with an optional background color.

Default

Block content.

Alert

Block content.

Example

Block content.

Default

Block content.

Alert

Block content.

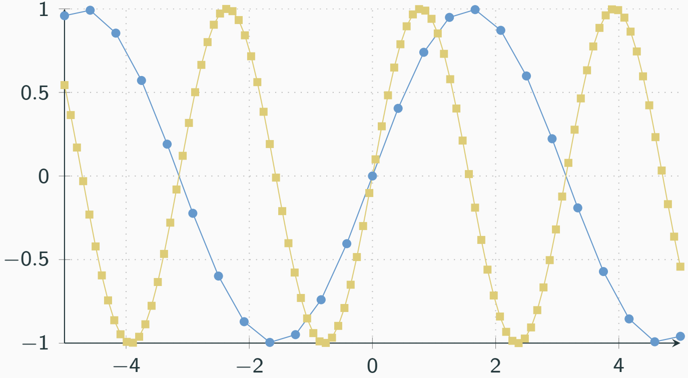
Example

Block content.

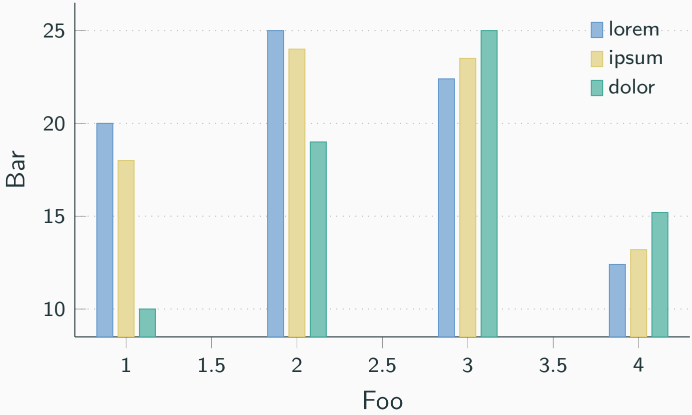
MATH

$$e = \lim_{n \to \infty} \left(1 + \frac{1}{n}\right)^n$$

LINE PLOTS



BAR CHARTS



QUOTES

Veni, Vidi, Vici

FRAME FOOTER

metropolis defines a custom beamer template to add a text to the footer. It can be set via

```
\setbeamertemplate{frame footer}{My custom footer}
```

REFERENCES

Some references to showcase [allowframebreaks] [**knuth92**, **ConcreteMath**, **Simpson**, **Er01**, **greenwade93**]

Conclusione

SUMMARY

Get the source of this theme and the demo presentation from

`github.com/matze/mtheme`

The theme *itself* is licensed under a Creative Commons Attribution-ShareAlike 4.0 International License.

Questions?

BACKUP SLIDES

Sometimes, it is useful to add slides at the end of your presentation to refer to during audience questions.

The best way to do this is to include the `appendixnumberbeamer` package in your preamble and call `\appendix` before your backup slides.

metropolis will automatically turn off slide numbering and progress bars for slides in the appendix.

References

- Giuseppe Carleo and Matthias Troyer. "Solving the quantum many-body problem with artificial neural networks". In: *Science* 355.6325 (2017), pp. 602–606. ISSN: 0036-8075. DOI: 10.1126/science.aag2302. eprint: http://science.sciencemag.org/content/355/6325/602.full.pdf. URL: http://science.sciencemag.org/content/355/6325/602.
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