Computational Quantum Mechanics

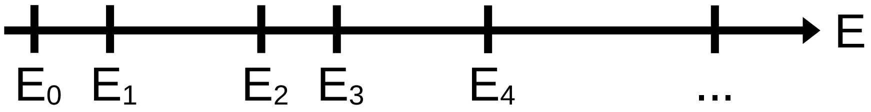
Prof. Gerson J. Ferreira

INFIS/UFU 2020/1

Variational Monte-Carlo

The variational method

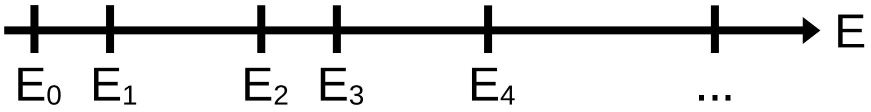
Let's assume H has the spectrum → where E0 corresponds to the lowest energy, all states satisfy



$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

The variational method

Let's assume H has the spectrum→ where E0 corresponds to the lowest energy, all states satisfy

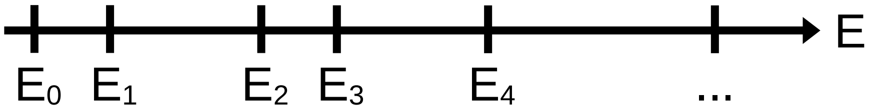


$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

Any other trial wave-function can be

The variational method

Let's assume H has the spectrum→ where E0 corresponds to the lowest energy, all states satisfy

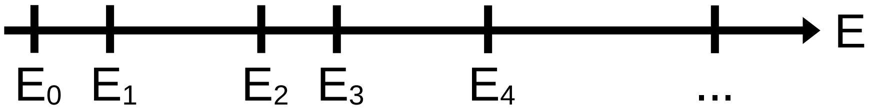


$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

Any other trial wave-function can be written as a linear combination→

The variational method

Let’s assume H has the spectrum→ where E0 corresponds to the lowest energy, all states satisfy

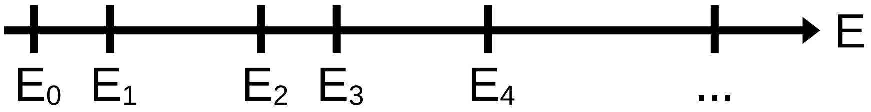


$$H\phi_n = E_n\phi_n \qquad \langle \phi_n | \phi_m \rangle = \delta_{n,m}$$

Any other trial wave-function can be written as a linear combination→ of the eigenstates,

The variational method

Let's assume H has the spectrum→ where E0 corresponds to the lowest energy, all states satisfy

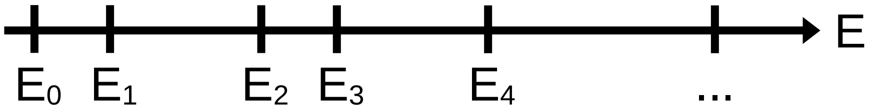


$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

Any other trial wave-function can be written as a linear combination→ of the eigenstates, and its energy is

The variational method

Let's assume H has the spectrum → where E0 corresponds to the lowest energy, all states satisfy



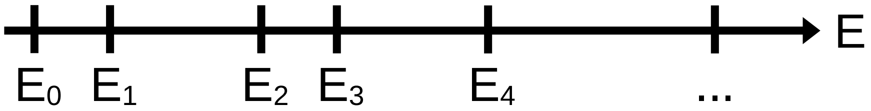
$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

Any other trial wave-function can be written as a linear combination → of the eigenstates, and its energy is

$$\psi = \sum_n c_n\phi_n$$

The variational method

Let's assume H has the spectrum →
where E0 corresponds to the lowest
energy, all states satisfy



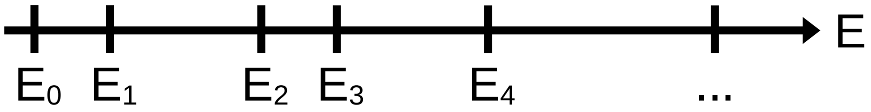
$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

Any other trial wave-function can be
written as a linear combination →
of the eigenstates,
and its energy is

$$\psi = \sum_n c_n\phi_n \qquad \langle\psi|\psi\rangle = \sum_n |c_n|^2 = 1$$

The variational method

Let's assume H has the spectrum → where E0 corresponds to the lowest energy, all states satisfy



$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

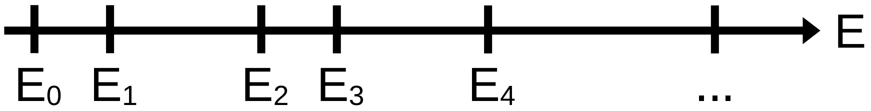
Any other trial wave-function can be written as a linear combination → of the eigenstates, and its energy is

$$\psi = \sum_n c_n\phi_n \qquad \langle\psi|\psi\rangle = \sum_n |c_n|^2 = 1$$

$$E = \langle\psi|H|\psi\rangle = \sum_n |c_n|^2 E_n = E_0 + \sum_n |c_n|^2 (E_n - E_0)$$

The variational method

Let's assume H has the spectrum →
where E0 corresponds to the lowest
energy, all states satisfy



$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

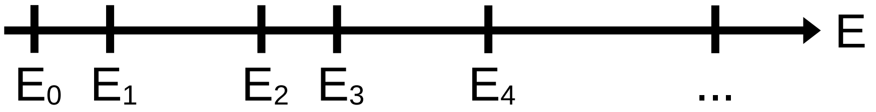
Any other trial wave-function can be
written as a linear combination →
of the eigenstates,
and its energy is

$$\psi = \sum_n c_n\phi_n \qquad \langle\psi|\psi\rangle = \sum_n |c_n|^2 = 1$$

$$E = \langle\psi|H|\psi\rangle = \sum_n |c_n|^2 E_n = E_0 + \underbrace{\sum_n |c_n|^2 (E_n - E_0)}_{>0}$$

The variational method

Let's assume H has the spectrum → where E0 corresponds to the lowest energy, all states satisfy



$$H\phi_n = E_n\phi_n \qquad \langle\phi_n|\phi_m\rangle = \delta_{n,m}$$

Any other trial wave-function can be be written as a linear combination → of the eigenstates, and its energy is

$$\psi = \sum_n c_n\phi_n \qquad \langle\psi|\psi\rangle = \sum_n |c_n|^2 = 1$$

$$E = \langle\psi|H|\psi\rangle = \sum_n |c_n|^2 E_n = E_0 + \underbrace{\sum_n |c_n|^2(E_n - E_0)}_{> 0}$$

$$\therefore E \geq E_0$$

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

Consider the effects of an infinitesimal change $\psi+\delta\psi$, and neglect $(\delta\psi)^2$ corrections

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

Consider the effects of an infinitesimal change ψ+δψ, and neglect (δψ)² corrections

$$E + \delta E = \frac{\langle\psi + \delta\psi|H|\psi + \delta\psi\rangle}{\langle\psi + \delta\psi|\psi + \delta\psi\rangle} = [E + \langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle]\left(\frac{1}{1 + \langle\psi|\delta\psi\rangle + \langle\delta\psi|\psi\rangle}\right)$$

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

Consider the effects of an infinitesimal change ψ+δψ, and neglect (δψ)² corrections

$$E + \delta E = \frac{\langle\psi + \delta\psi|H|\psi + \delta\psi\rangle}{\langle\psi + \delta\psi|\psi + \delta\psi\rangle} = [E + \langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle] \underbrace{\left(\frac{1}{1 + \langle\psi|\delta\psi\rangle + \langle\delta\psi|\psi\rangle}\right)}_{\frac{1}{1+x} \approx 1 - x}$$

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

Consider the effects of an infinitesimal change ψ+δψ, and neglect (δψ)² corrections

$$E + \delta E = \frac{\langle\psi + \delta\psi|H|\psi + \delta\psi\rangle}{\langle\psi + \delta\psi|\psi + \delta\psi\rangle} = [E + \langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle]\underbrace{\left(\frac{1}{1 + \langle\psi|\delta\psi\rangle + \langle\delta\psi|\psi\rangle}\right)}_{\frac{1}{1+x} \approx 1 - x}$$

Neglect (δψ)² corrections again to get

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

Consider the effects of an infinitesimal change ψ+δψ, and neglect $(\delta\psi)^2$ corrections

$$E + \delta E = \frac{\langle\psi + \delta\psi|H|\psi + \delta\psi\rangle}{\langle\psi + \delta\psi|\psi + \delta\psi\rangle} = [E + \langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle]\underbrace{\left(\frac{1}{1 + \langle\psi|\delta\psi\rangle + \langle\delta\psi|\psi\rangle}\right)}_{\frac{1}{1+x} \approx 1 - x}$$

Neglect $(\delta\psi)^2$ corrections again to get

$$\delta E = \langle\psi|H - E|\psi + \delta\psi\rangle + \langle\psi + \delta\psi|H - E|\psi\rangle + \mathcal{O}(\delta\psi^2)$$

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

Consider the effects of an infinitesimal change ψ+δψ, and neglect $(\delta\psi)^2$ corrections

$$E + \delta E = \frac{\langle\psi+\delta\psi|H|\psi+\delta\psi\rangle}{\langle\psi+\delta\psi|\psi+\delta\psi\rangle} = [E + \langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle]\underbrace{\left(\frac{1}{1+\langle\psi|\delta\psi\rangle+\langle\delta\psi|\psi\rangle}\right)}_{\frac{1}{1+x}\approx 1-x}$$

Neglect $(\delta\psi)^2$ corrections again to get

$$\delta E = \langle\psi|H-E|\psi+\delta\psi\rangle + \langle\psi+\delta\psi|H-E|\psi\rangle + \mathcal{O}(\delta\psi^2)$$

But if ψ is the eigenstate with energy E, then δE = 0

Local minima

Assuming: $H|\psi\rangle = E|\psi\rangle \qquad \langle\psi|\psi\rangle = 1$

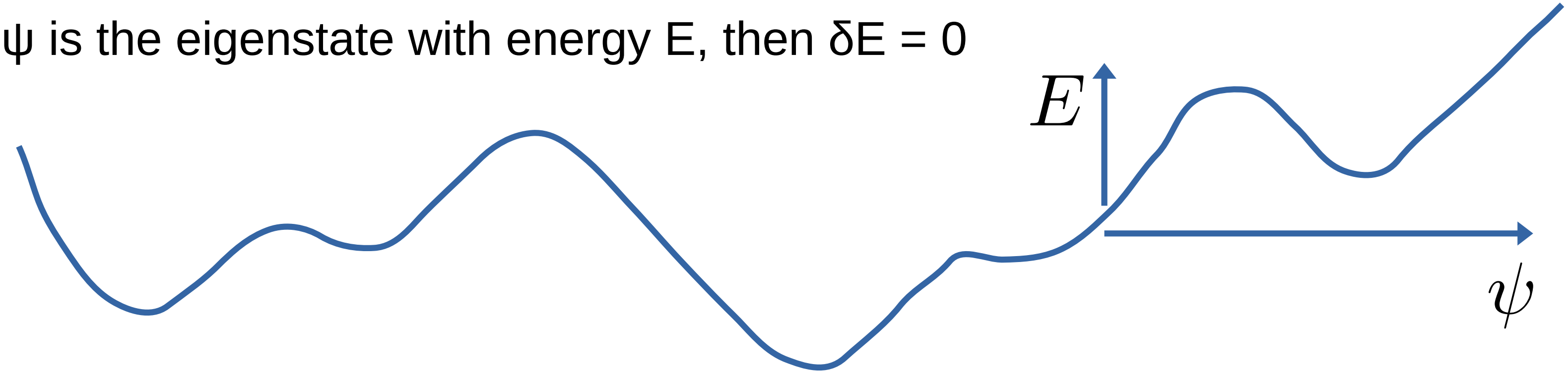
Consider the effects of an infinitesimal change ψ+δψ, and neglect (δψ)² corrections

$$E + \delta E = \frac{\langle\psi + \delta\psi|H|\psi + \delta\psi\rangle}{\langle\psi + \delta\psi|\psi + \delta\psi\rangle} = [E + \langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle] \underbrace{\left(\frac{1}{1 + \langle\psi|\delta\psi\rangle + \langle\delta\psi|\psi\rangle}\right)}_{\frac{1}{1+x} \approx 1 - x}$$

Neglect (δψ)² corrections again to get

$$\delta E = \langle\psi|H - E|\psi + \delta\psi\rangle + \langle\psi + \delta\psi|H - E|\psi\rangle + \mathcal{O}(\delta\psi^2)$$

But if ψ is the eigenstate with energy E, then δE = 0



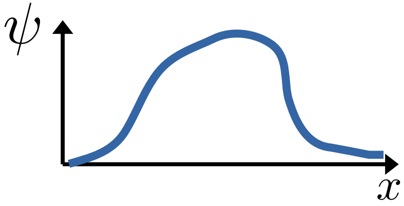
Variational Monte-Carlo

Now we know that any trial wave-function satisfies: $E = \langle\psi|H|\psi\rangle \geq E_0$

Variational Monte-Carlo

Now we know that any trial wave-function satisfies: $E = \langle\psi|H|\psi\rangle \geq E_0$

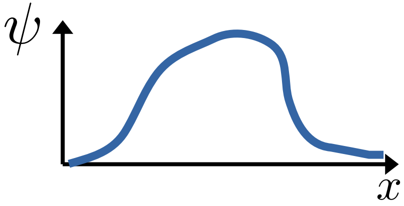
1) Guess an initial trial function



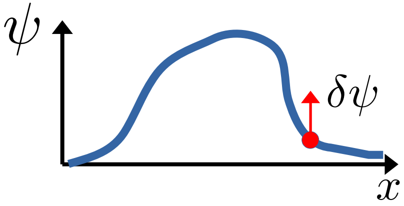
Variational Monte-Carlo

Now we know that any trial wave-function satisfies: $E = \langle \psi | H | \psi \rangle \geq E_0$

1) Guess an initial trial function



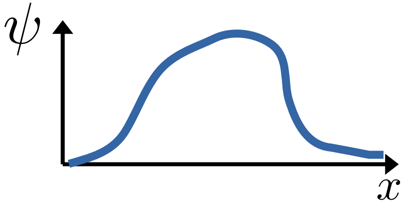
2) Sample a random point and make a small change



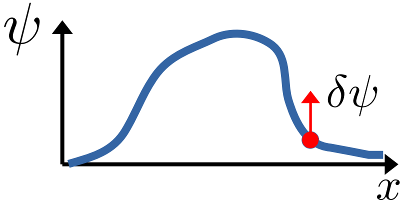
Variational Monte-Carlo

Now we know that any trial wave-function satisfies: $E = \langle\psi|H|\psi\rangle \geq E_0$

1) Guess an initial trial function



2) Sample a random point and make a small change



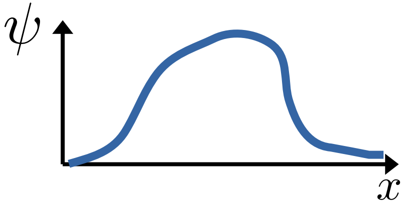
3) Calculate the new energy

$$E(\delta\psi) = \frac{\langle\psi+\delta\psi|H|\psi+\delta\psi\rangle}{\langle\psi+\delta\psi|\psi+\delta\psi\rangle}$$

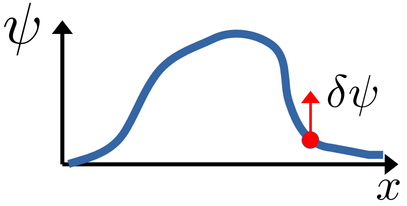
Variational Monte-Carlo

Now we know that any trial wave-function satisfies: $E = \langle \psi | H | \psi \rangle \geq E_0$

1) Guess an initial trial function



2) Sample a random point and make a small change



3) Calculate the new energy

$$E(\delta\psi) = \frac{\langle \psi + \delta\psi | H | \psi + \delta\psi \rangle}{\langle \psi + \delta\psi | \psi + \delta\psi \rangle}$$

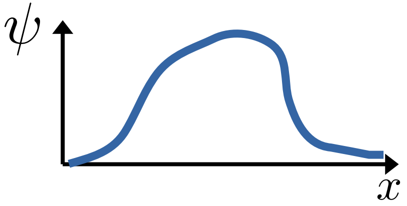
4) If new E < old E, accept else, reject the change.

Return to step 2 and loop until convergence (?)

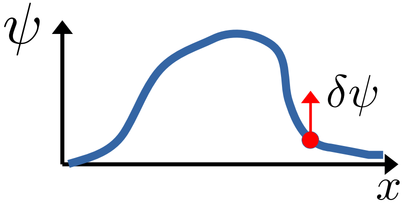
Variational Monte-Carlo

Now we know that any trial wave-function satisfies: $E = \langle\psi|H|\psi\rangle \geq E_0$

1) Guess an initial trial function



2) Sample a random point and make a small change



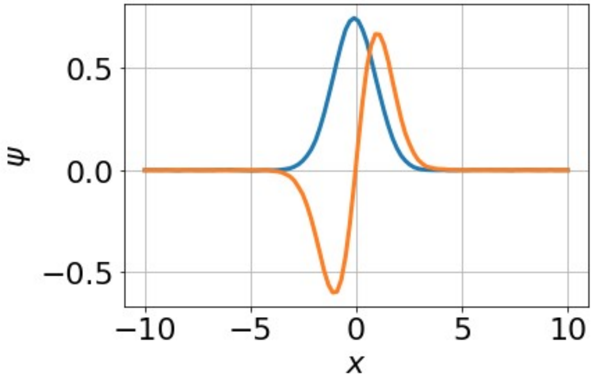
3) Calculate the new energy

$$E(\delta\psi) = \frac{\langle\psi + \delta\psi|H|\psi + \delta\psi\rangle}{\langle\psi + \delta\psi|\psi + \delta\psi\rangle}$$

4) If new E < old E, accept else, reject the change.

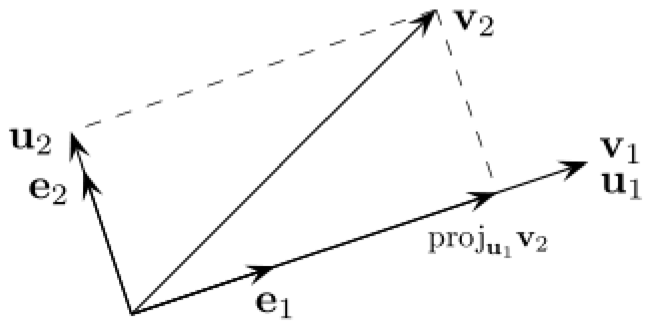
Return to step 2 and loop until convergence (?)

The result



Gram-Schmidt orthogonalization

Simple process to orthogonalize a set of vectors

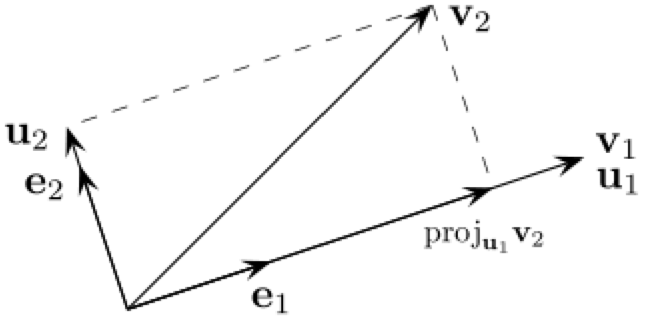


(see Wikipedia for better implementations)

Gram-Schmidt orthogonalization

Simple process to orthogonalize a set of vectors

1) Let's define the projection of v into u as: $\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$



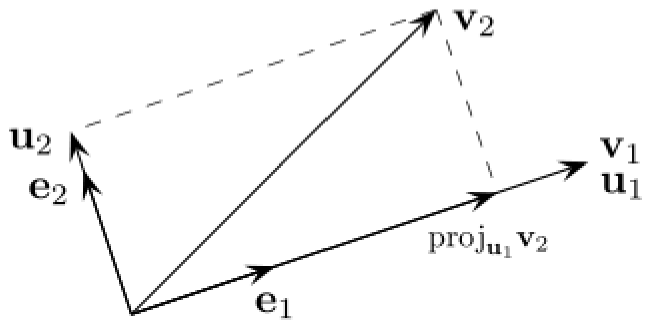
(see Wikipedia for better implementations)

Gram-Schmidt orthogonalization

Simple process to orthogonalize a set of vectors

1) Let's define the projection of v into u as: $\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$

2) Say that we want to orthogonalize the set $\{v_1, v_2, v_3\}$.



(see Wikipedia for better implementations)

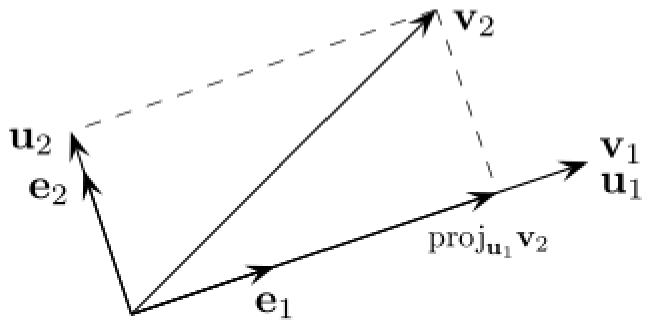
Gram-Schmidt orthogonalization

Simple process to orthogonalize a set of vectors

1) Let's define the projection of v into u as: $\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$

2) Say that we want to orthogonalize the set $\{v_1, v_2, v_3\}$.

→ let's start with v1, and subtract it's projection from v2, and so on...



(see Wikipedia for better implementations)

Gram-Schmidt orthogonalization

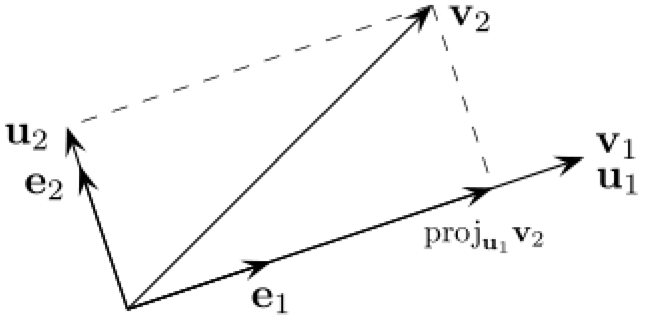
Simple process to orthogonalize a set of vectors

1) Let's define the projection of v into u as: $\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$

2) Say that we want to orthogonalize the set {v_1, v_2, v_3}.

→ let's start with v1, and subtract it's projection from v2, and so on...

$$u_1 = v_1$$



(see Wikipedia for better implementations)

Gram-Schmidt orthogonalization

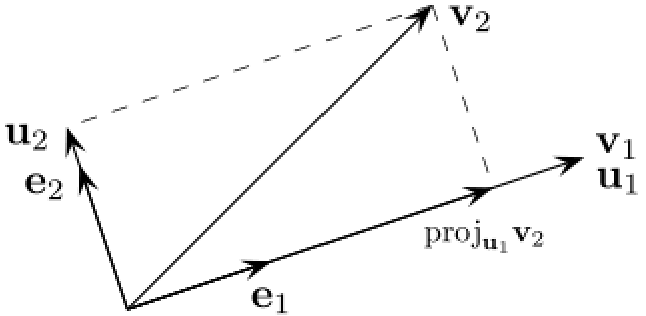
Simple process to orthogonalize a set of vectors

1) Let's define the projection of v into u as: $\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$

2) Say that we want to orthogonalize the set $\{v_1, v_2, v_3\}$.

→ let's start with v1, and subtract it's projection from v2, and so on...

$$u_1 = v_1$$
$$u_2 = v_2 - \mathrm{proj}_{u_1}(v_2)$$



(see Wikipedia for better implementations)

Gram-Schmidt orthogonalization

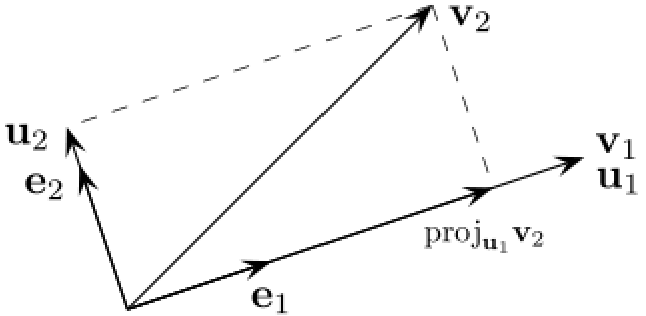
Simple process to orthogonalize a set of vectors

1) Let's define the projection of v into u as: $\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$

2) Say that we want to orthogonalize the set $\{v_1, v_2, v_3\}$.

→ let's start with v1, and subtract it's projection from v2, and so on...

$$u_1 = v_1$$
$$u_2 = v_2 - \mathrm{proj}_{u_1}(v_2)$$
$$u_3 = v_3 - \mathrm{proj}_{u_1}(v_3) - \mathrm{proj}_{u_2}(v_3)$$



(see Wikipedia for better implementations)

Gram-Schmidt orthogonalization

Simple process to orthogonalize a set of vectors

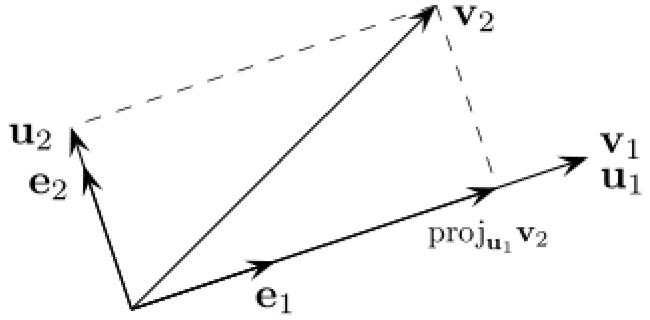
1) Let's define the projection of v into u as: $\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$

2) Say that we want to orthogonalize the set $\{v_1, v_2, v_3\}$.

→ let's start with v1, and subtract it's projection from v2, and so on...

$$
\begin{aligned}
u_1 &= v_1 \\
u_2 &= v_2 - \mathrm{proj}_{u_1}(v_2) \\
u_3 &= v_3 - \mathrm{proj}_{u_1}(v_3) - \mathrm{proj}_{u_2}(v_3)
\end{aligned}
$$

3) Normalize the new set $\{u_1, u_2, u_3\}$ at the end only



(see Wikipedia for better implementations)

Gram-Schmidt orthogonalization: example

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

$$\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \mathrm{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \mathrm{proj}_{u_1}(v_3) - \mathrm{proj}_{u_2}(v_3)$$

Gram-Schmidt orthogonalization: example

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

1) u1 = (1, 0, 0)

$$\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \mathrm{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \mathrm{proj}_{u_1}(v_3) - \mathrm{proj}_{u_2}(v_3)$$

Gram-Schmidt orthogonalization: example

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

1) u1 = (1, 0, 0)

2) $\text{proj}_{u1}(v2)$ = (1, 0, 0) → u2 = (0, 1, 1)

$$\text{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle}u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \text{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \text{proj}_{u_1}(v_3) - \text{proj}_{u_2}(v_3)$$

Gram-Schmidt orthogonalization: example

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

1) u1 = (1, 0, 0)

2) $\text{proj}_{u1}(v2)$ = (1, 0, 0) → u2 = (0, 1, 1)

3) $\text{proj}_{u1}(v3)$ = (2, 0, 0) & $\text{proj}_{u2}(v3)$ = (0, -½, -½)

$$\text{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \text{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \text{proj}_{u_1}(v_3) - \text{proj}_{u_2}(v_3)$$

Gram-Schmidt orthogonalization: example

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

1) u1 = (1, 0, 0)

2) proj_{u1}(v2) = (1, 0, 0) → u2 = (0, 1, 1)

3) proj_{u1}(v3) = (2, 0, 0) & proj_{u2}(v3) = (0, -½, -½)
→ u3 = (2, -1, 0) – (2, 0, 0) – (0, -½, -½)

$$\text{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \text{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \text{proj}_{u_1}(v_3) - \text{proj}_{u_2}(v_3)$$

Gram-Schmidt orthogonalization: example

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

1) u1 = (1, 0, 0)

2) proj_{u1}(v2) = (1, 0, 0) → u2 = (0, 1, 1)

3) proj_{u1}(v3) = (2, 0, 0) & proj_{u2}(v3) = (0, -½, -½)
→ u3 = (2, -1, 0) – (2, 0, 0) – (0, -½, -½)
→ u3 = (0, -½, ½)

$$\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \mathrm{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \mathrm{proj}_{u_1}(v_3) - \mathrm{proj}_{u_2}(v_3)$$

Gram-Schmidt orthogonalization: example

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

1) u1 = (1, 0, 0)

2) $\text{proj}_{u1}(v2) = (1, 0, 0) \rightarrow u2 = (0, 1, 1)$

3) $\text{proj}_{u1}(v3) = (2, 0, 0)$ & $\text{proj}_{u2}(v3) = (0, -½, -½)$

→ u3 = (2, -1, 0) – (2, 0, 0) – (0, -½, -½)

→ u3 = (0, -½, ½)

4) normalize to get

$$\text{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle} u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \text{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \text{proj}_{u_1}(v_3) - \text{proj}_{u_2}(v_3)$$

Gram-Schmidt orthogonalization: example

$$\mathrm{proj}_u(v) = \frac{\langle u|v\rangle}{\langle u|u\rangle}u$$

$$u_1 = v_1$$

$$u_2 = v_2 - \mathrm{proj}_{u_1}(v_2)$$

$$u_3 = v_3 - \mathrm{proj}_{u_1}(v_3) - \mathrm{proj}_{u_2}(v_3)$$

V1 = (1, 0, 0)
V2 = (1, 1, 1)
V3 = (2, -1, 0)

1) u1 = (1, 0, 0)

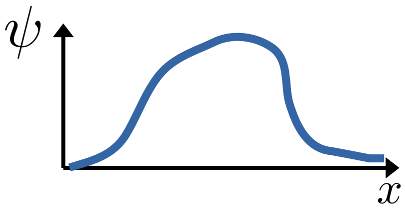
2) proj_{u1}(v2) = (1, 0, 0) → u2 = (0, 1, 1)

3) proj_{u1}(v3) = (2, 0, 0) & proj_{u2}(v3) = (0, -½, -½)
→ u3 = (2, -1, 0) – (2, 0, 0) – (0, -½, -½)
→ u3 = (0, -½, ½)

4) normalize to get

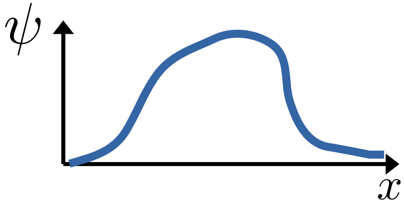
$$u_1 = (1, 0, 0) \qquad u_2 = \frac{1}{\sqrt{2}}(0, 1, 1) \qquad u_3 = \frac{1}{\sqrt{2}}(0, -1, 1)$$

Importance sampling



Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

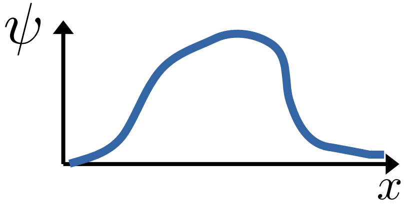
Importance sampling



Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

The rejection method

Importance sampling

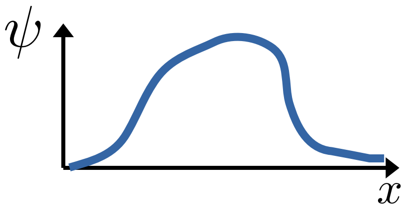


Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

The rejection method

- Sample a random x

Importance sampling



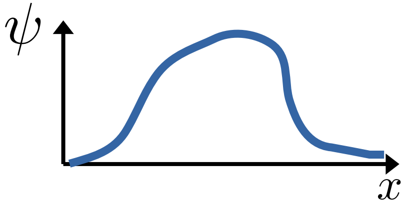
Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

The rejection method

- Sample a random x
- Let P = $|\psi(x)|^2$ will be the probability to accept x

  → Normalize P by the maximum value of $|\psi(x)|^2$

Importance sampling



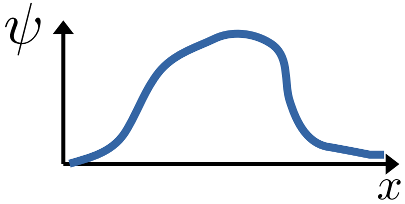
Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

The rejection method

- Sample a random x
- Let $P = |\psi(x)|^2$ will be the probability to accept x

  → Normalize P by the maximum value of $|\psi(x)|^2$
- Sample an uniform number $0 < q < 1$

Importance sampling



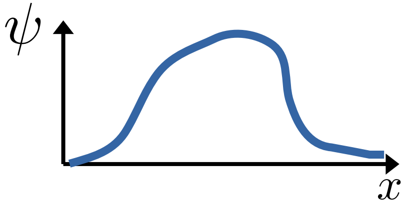
Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

<u>The rejection method</u>

- Sample a random x
- Let P = $|\psi(x)|^2$ will be the probability to accept x

  → Normalize P by the maximum value of $|\psi(x)|^2$
- Sample an uniform number $0 < q < 1$
- Accept if $q > P$

Importance sampling



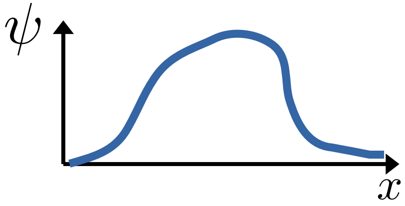
Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

<u>The rejection method</u>

- Sample a random x
- Let P = $|\psi(x)|^2$ will be the probability to accept x

  → Normalize P by the maximum value of $|\psi(x)|^2$
- Sample an uniform number $0 < q < 1$
- Accept if $q > P$
- Otherwise try a different x

Importance sampling



Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

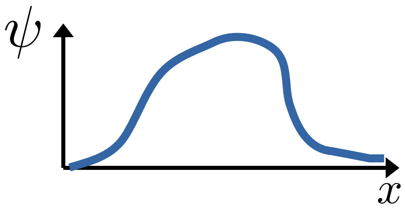
The rejection method

- Sample a random x
- Let P = $|\psi(x)|^2$ will be the probability to accept x

  → Normalize P by the maximum value of $|\psi(x)|^2$
- Sample an uniform number 0 < q < 1
- Accept if q > P
- Otherwise try a different x

Exercise:

Importance sampling



Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

The rejection method

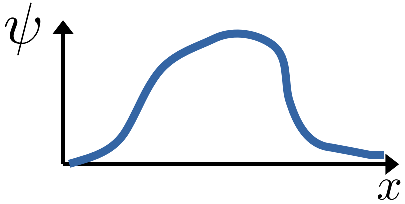
- Sample a random x
- Let P = $|\psi(x)|^2$ will be the probability to accept x

  → Normalize P by the maximum value of $|\psi(x)|^2$
- Sample an uniform number $0 < q < 1$
- Accept if $q > P$
- Otherwise try a different x

Exercise:

→ Write a code to sample points with a Gaussian distribution P(x) within the interval $-5<x<5$.

Importance sampling



Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

<u>The rejection method</u>

- Sample a random x
- Let P = $|\psi(x)|^2$ will be the probability to accept x

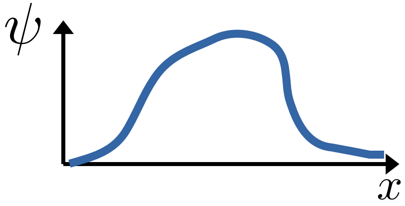
  → Normalize P by the maximum value of $|\psi(x)|^2$
- Sample an uniform number 0 < q < 1
- Accept if q > P
- Otherwise try a different x

<u>Exercise:</u>

→ Write a code to sample points with a Gaussian distribution P(x) within the interval -5<x<5.

→ Plot the histogram with

Importance sampling



Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

The rejection method

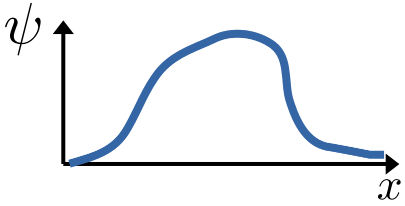
- Sample a random x
- Let P = $|\psi(x)|^2$ will be the probability to accept x
  - → Normalize P by the maximum value of $|\psi(x)|^2$
- Sample an uniform number $0 < q < 1$
- Accept if $q > P$
- Otherwise try a different x

Exercise:

→ Write a code to sample points with a Gaussian distribution P(x) within the interval $-5<x<5$.

→ Plot the histogram with
plt.hist(points)

Importance sampling



Small changes in regions where ψ is small, won't affect E.
It's better to focus on regions where ψ is large.

The rejection method

- Sample a random x
- Let P = |ψ(x)|² will be the probability to accept x
  → Normalize P by the maximum value of |ψ(x)|²
- Sample an uniform number 0 < q < 1
- Accept if q > P
- Otherwise try a different x

Exercise:

→ Write a code to sample points with a Gaussian distribution P(x) within the interval -5<x<5.

→ Plot the histogram with plt.hist(points)