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Solving linear equations on an adiabatic quantum computer (AQC)

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Sochi, 2021

Adiabatic quantum algorithm

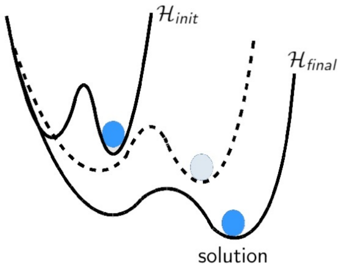
The Hamiltonian of the system is equal to the energy of the system.

- $\mathcal{H}_{init}(\sigma)$ is an initial Hamiltonian, σ is a state of the system.
- $\mathcal{H}_{final}(\sigma)$ is a final Hamiltonian encoding the solution of some problem.

Evolution of $\mathcal{H}_{init}$ into $\mathcal{H}_{final}$ is an evolution of the system with the Hamiltonian

$$\mathcal{H}(t) = (1 - t/T)\mathcal{H}_{init} + (t/T)\mathcal{H}_{final},$$

where T is the time of system evolution.



Types of the final Hamiltonian

Ising problem

$$H_{ising}(\mathbf{s}) = \sum_{i=1}^{N} h_i s_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} J_{ij} s_i s_j,$$

$s_i \in \{+1, -1\},\ J_{ij}, h_i \in \mathbb{R}$

QUBO problem

$$H_{qubo}(\mathbf{q}) = \sum_{i=1}^{N} h_i q_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} J_{ij} q_i q_j = \sum_{i=1}^{N} \sum_{j=i}^{N} J_{ij} q_i q_j,$$

$q_i \in \{0, 1\},\ J_{ij}, h_i \in \mathbb{R},\ J_{ii} = h_i,\ (q_i^2 = q_i).$

The main idea

The desired solution of some problem is the point where H has its global minimum.

The problem

- We consider a one-dimensional equation $ax = b$.
- Construct a final Hamiltonian $H(x) = (ax - b)^2$ whose minimum point is b/a.
- Represent the variable as $x = c\chi - d$, where $\chi = \sum_{i=0}^{R-1} 2^{-i} q_i \in [0, 2)$ with $\forall q_i \in \{0, 1\}$ and $c, d > 0$.
- Hence $x \in [-d, 2c - d)$
- The Hamiltonian with variables q_i has the form

$$H(q_0, \ldots, q_{R-1}) = \sum_{i=0}^{R-1} h_i q_i + \sum_{i=0}^{R-1} \sum_{j=i+1}^{R-1} J_{ij} q_i q_j$$

$$h_i = 2^{-i} ac \left(2^{-i} ac - 2(ad + b)\right)$$
$$J_{ij} = 2a^2 c^2 2^{-i-j}$$

D-Wave's computers

D-Wave 2000Q (2041 qubits)

Advantage System (5627 qubits)

Probabilistic nature of adiabatic quantum computers

Boltzmann distribution (BD)

Let $H(x)$ be a Hamiltonian of the system,
$x_1, \ldots, x_N$ be all possible states of the system.
Then the probability that the system is in the state x_k

$$P(x_k) = \frac{1}{Q} e^{-\beta H(x_k)},$$

where $Q = \sum e^{-\beta H(x_j)}$, $\beta = \frac{1}{k_B T}$ is the parameter of the distribution, k_B is the Boltzmann constant, T is the thermodynamic temperature of the system. We will omit physical nature of the parameter β in further considerations.

The limit distribution

If the number of states of the system tends to infinity and the states become more dense then the distribution becomes normal.

Statement

1) Let X_n be a random variable such that

$$X_n \in \Omega_n = \left\{ \pm \sum_{i=-n}^{n-1} q_i \, 2^i \;\middle|\; q_i \in \{0,1\} \right\} \subset \mathbb{R}.$$

2) Let P_n be a probability measure on Ω_n such that

$$P_n(x) = P_n(X_n = x) \propto e^{-\beta H(x)},$$

where $H(x) = (ax-b)^2$, $\beta > 0$. Then

$$X_n \xrightarrow{\mathcal{D}} N\left(\frac{b}{a}, \frac{1}{a\sqrt{2\beta}}\right), \quad n \to \infty$$

Proof

- We let $\mu_n(A) := \sum_{x_k \in \Omega_n} P_n(x_k)\delta_x(A)$ be a measure on $\mathbb{R}$ where
- $P_n(x_k) = \frac{1}{Q_n} e^{-\beta(ax_k - b)^2}, \ Q_n = \sum_{x_i \in \Omega_n} e^{-\beta(ax_i - b)^2}$
- We then compute an asymptotic formula for Q_n

$$Q_n = 2^n \sum_{x_i \in \Omega_n} \frac{1}{2^n} e^{-\beta(ax_i - b)^2}$$

$$\sim 2^n \int_{-\infty}^{\infty} e^{-\beta(at - b)^2} dt = \frac{2^n \sqrt{\pi}}{a\sqrt{\beta}}$$

- Now we can calculate the limit of μ_n

$$\mu_n(A) = \frac{1}{Q_n} \sum_{x_k \in \Omega_n} e^{-\beta(ax_k - b)^2} \cdot \delta_{x_k}(A)$$

$$\xrightarrow{n \to \infty} \frac{a\sqrt{\beta}}{\sqrt{\pi}} \int_A e^{-\beta(at - b)^2} dt = \frac{1}{\sigma\sqrt{2\pi}} \int_A e^{-\frac{(t - b/a)^2}{2\sigma^2}} dt, \quad \sigma = \frac{1}{a\sqrt{2\beta}}$$

Parameters of the distribution of solutions

Normal distribution

- Let $F_\sigma(x) = \frac{1}{\sigma\sqrt{2\pi}} \int\limits_{-\infty}^{x} e^{-\frac{(t-b/a)^2}{2\sigma^2}} dt$ be the CDF of the limit normal distribution, $\sigma = \frac{1}{a\sqrt{2\beta}}$
- Let $F_N(x)$ be the eCDF of a sample then

$$\hat{\sigma} = \arg\min_{\sigma} \|F_\sigma(x) - F_N(x)\|_{L^2}$$

Boltzmann distribution

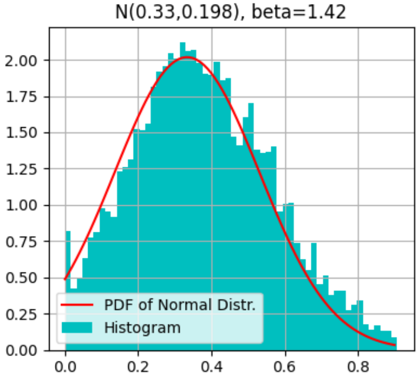
- Let Q be the BD, q_i be the probability of x_i,
- Let P be the empirical distribution, p_i be the frequency of x_i.

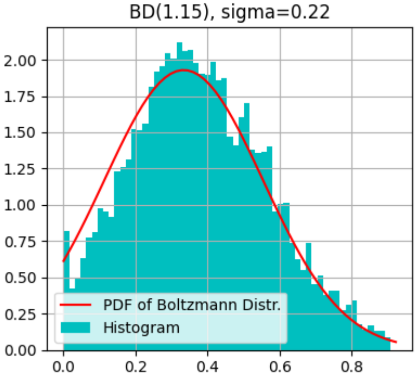
$$\hat{\beta} = \arg\min_{\beta} \mathrm{JSD}(P||Q)$$

$\mathrm{JSD}(P||Q) = \frac{1}{2}D_{KL}(P||M) + \frac{1}{2}D_{KL}(Q||M)$, $M = \frac{1}{2}(P+Q)$, e.g. $D_{KL}(P||Q) = \sum_i p_i \log \frac{p_i}{q_i}$

Examples

- $3x = 1$
- $x = \chi = \sum_{i=0}^{R-1} 2^{-i} q_i \Rightarrow x \in [0, 2)$, we use $\sigma = \frac{1}{a\sqrt{2\beta}}$, $R = 7$

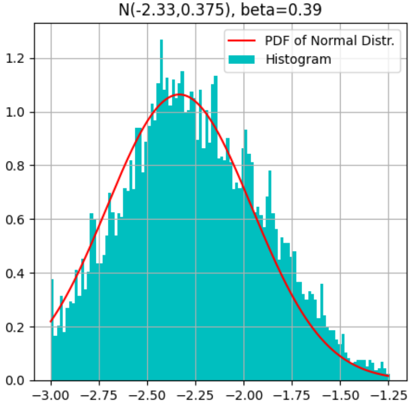


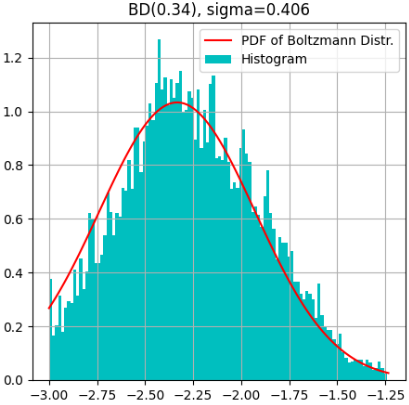


- The best solution is 0.328
- Sample mean is 0.387

Examples

- $3x = -5$
- $x = 2\chi - 3 \in [-3, 1), \;\; R = 8$





- The best solution is -2.328
- Sample mean is -2.246

Improving the solution

- Let x_k be an approximate solution of $ax = b$
- The exact solution $x = x_k + \Delta_k$
- The equation for Δ_k is $a\Delta_k = b - ax_k$,
- The next approximation to the solution is $x_{k+1} = x_k + \Delta_k$
- Assume $\Delta_k \sim N\left(\frac{b-ax_k}{a}, \frac{1}{a\sqrt{2\beta}}\right)$, according to the statement about the limit distribution
- Then x_k does not converge to $\frac{b}{a}$

Improving the solution

Another scheme

- Let $a \in \left(\frac{1}{2}, 1\right)$ and $\widetilde{\Delta}_k = 2^l \Delta_k$ such that $|\widetilde{\Delta}_k| \in \left(\frac{1}{2}, 1\right)$
- Equation for $\widetilde{\Delta}_k$ then is $a\widetilde{\Delta}_k = 2^l(b - ax_k)$
- The same assumption gives $\Delta_k \sim \frac{1}{2^l} N\left(\frac{2^l(b-ax_k)}{a}, \frac{1}{a\sqrt{2\beta}}\right)$
- If $a \in \left(\frac{1}{2}, 1\right)$ then $|b - ax_k| \in \left(\frac{1}{2^{l+2}}, \frac{1}{2^l}\right)$ but assume $|b - ax_k| \approx \frac{1}{2^l}$
- Thus we can write $\Delta_k \sim (b - ax_k)N\left(\frac{1}{a}, \frac{1}{a\sqrt{2\beta}}\right)$
- Then $x_{k+1} = x_k + \Delta_k$ does converge to $\frac{b}{a}$

Improving the solution

Theorem (convergence of the approximations)

Let $x_0 = 0$, $x_{k+1} = x_k + \Delta_k$ for $k \geqslant 0$, where Δ_k is a random variable distributed as $(b - ax_k)N\left(\frac{1}{a}, \sigma\right)$, where $a > 0, b \in \mathbb{R}$. Then $x_k \to \frac{b}{a}$ in probability as $k \to \infty$ if $a\sigma < \sqrt{2}\, e^{\frac{\gamma}{2}}$, where $\gamma \approx 0.577$ is the Euler-Mascheroni constant.

It can be reformulated if $\sigma = \frac{1}{a\sqrt{2\beta}}$ then the condition $a\sigma < \sqrt{2}\, e^{\frac{\gamma}{2}}$ becomes $\beta > \frac{1}{4}e^{-\gamma}$

Proof of the theorem

Consider $z_k = x_k - \frac{b}{a}$ and prove $z_k \xrightarrow{P} 0$. Denote $\xi_k \sim N\left(\frac{1}{a}, \sigma\right)$. We can simply derive the recurrence relation for z_k

$$z_k = -(a\xi_{k-1} - 1)z_{k-1} = -\zeta_{k-1}z_{k-1}$$

where $\zeta_k \sim N(0, a\sigma)$. Since $z_0 = -\frac{b}{a}$ then

$$z_k = (-1)^{k+1}\frac{b}{a}\zeta_0\zeta_1 \dots \zeta_{k-1}$$

Taking log of the above relation we get

$$\log|z_k| = \log\left|\frac{b}{a}\right| + \log|\zeta_0| + \log|\zeta_1| + \dots + \log|\zeta_{k-1}|$$

Next we find an expectation of $\log|\zeta_i|$

Proof of the theorem

Omitting details of calculations of an integral we get

$$\mathbb{E} \log |\zeta_i| = \log \frac{a\sigma}{\sqrt{2}} - \frac{\gamma}{2}$$

(we use here a nice equality $\int\limits_0^\infty e^{-x^2} \log x \, dx = -\frac{1}{4}\sqrt{\pi}\,(\gamma + 2\log 2)$)

Since $a\sigma < \sqrt{2}e^{\frac{\gamma}{2}}$ then $\mathbb{E} \log |\zeta_i| < 0$. So by Law of large numbers we have

$$\frac{1}{k}\left(\log|\zeta_0| + \log|\zeta_1| + \ldots + \log|\zeta_{k-1}|\right) \xrightarrow{P} \log \frac{a\sigma}{\sqrt{2}} - \frac{\gamma}{2} < 0$$

Hence $\log\left|\frac{b}{a}\right| + \log|\zeta_0| + \ldots + \log|\zeta_{k-1}| \xrightarrow{P} -\infty$ exponentiating we get $|z_k| \xrightarrow{P} 0$.

Speed of convergence

Statement

Let $x_0 = 0$, $x_{k+1} = x_k + \Delta_k$, *where* $\Delta_k \sim (b - a x_k) N\left(\frac{1}{a}, \sigma\right)$ *and* $a\sigma < \sqrt{2}\, e^{\frac{\gamma}{2}}$. *Let*

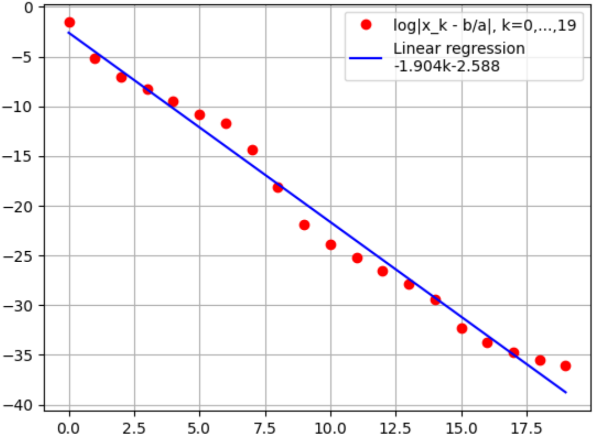
$$s_k = \left(\frac{\sqrt{2}\, e^{\gamma/2-\delta}}{a\sigma}\right)^k = \left(2\sqrt{\beta e^{\gamma-2\delta}}\right)^k$$

where $\delta > 0$. *Then* $\left(x_k - \frac{b}{a}\right) s_k \xrightarrow{P} 0$.

- Let $\delta = 0$ and assume $s_k \left|x_k - \frac{b}{a}\right| \approx 1$
- So $\left|x_k - \frac{b}{a}\right| \approx e^{\rho k}$ such that $\left(e^{\rho} \cdot 2\sqrt{\beta e^{\gamma}}\right)^k \approx 1$
- Hence $\beta \approx \frac{1}{4e^{\gamma+2\rho}}$

Speed of convergence

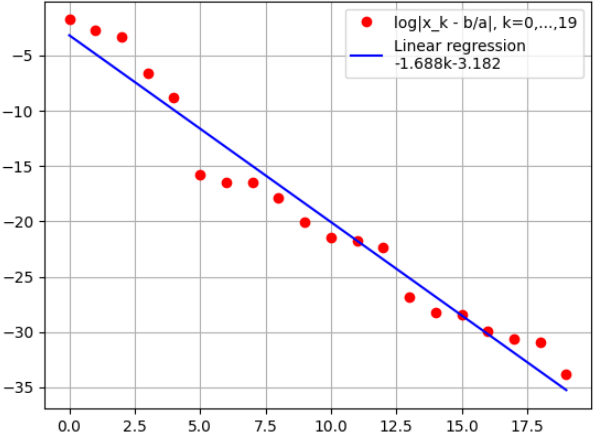
- $0.75x = 0.25$
- On each step we are in $[-1, 1)$ and $R = 10$



- $\beta = 6.32$

Speed of convergence

- $0.875x = -0.625$
- On each step we are in $[-1, 1)$ and $R = 10$



- $\beta = 4.1$

The case of a truncated normal distribution

Limit distribution

- It the statement about the limit distribution of solutions X_n was a random variable which took values from $\Omega_n = \left\{\pm \sum_{i=-n}^{n} q_i \, 2^i \,\middle|\, q_i \in \{0,1\}\right\} \subset \mathbb{R}$
- Now let $X_n \in \Omega_n = \left\{\pm \sum_{i=-n}^{n-1} q_i \, 2^i \in (r_1, r_2) \,\middle|\, q_i \in \{0,1\}\right\}$, $r_1 < r_2 \in \mathbb{R}$
- As before $P_n(X_n = x) \propto e^{-\beta(ax-b)^2}$ — Boltzmann distribution over Ω_n
- Then $X_n \xrightarrow{\mathcal{D}} N\left(\frac{b}{a}, \frac{1}{a\sqrt{2\beta}}, r_1, r_2\right)$ which has the density

$$p(t) = \frac{1}{\sigma\sqrt{2\pi}Q} e^{-\frac{(t-b/a)^2}{2\sigma^2}} \mathbf{1}_{(r_1,r_2)}(t),$$

where $Q = \Phi\left(\frac{r_2 - b/a}{\sigma}\right) - \Phi\left(\frac{r_1 - b/a}{\sigma}\right)$ and $\sigma = \frac{1}{a\sqrt{2\beta}}$

Case of a truncated normal distribution

Improving the solution

- Let x_k be an approximate solution of $ax = b$, then the exact solution is $x = x_k + \Delta_k$
- The equation for Δ_k is $a\Delta_k = b - ax_k$, the next approximation to the solution is $x_{k+1} = x_k + \Delta_k$
- Assume $\Delta_k \sim N\left(\frac{b-ax_k}{a}, \sigma, \frac{b-ax_k}{a}(1 \pm \varepsilon)\right)$, where $\sigma = \frac{1}{a\sqrt{2\beta}}$, $\varepsilon > 0$
- $\widetilde{\Delta}_k = 2^l \Delta_k$ such that $|\widetilde{\Delta}_k| \in \left(\frac{1}{2}, 1\right)$, then $a\widetilde{\Delta}_k = 2^l(b - ax_k)$
- Hence $\Delta_k \sim \frac{1}{2^l}\widetilde{N}\left(\frac{2^l(b-ax_k)}{a}, \sigma, \frac{2^l(b-ax_k)}{a}(1 \pm \varepsilon)\right)$
- If $a \in \left(\frac{1}{2}, 1\right)$ then $|b - ax_k| \in \left(\frac{1}{2^{l+2}}, \frac{1}{2^l}\right) \Rightarrow |b - ax_k| \approx \frac{1}{2^l}$
- Thus $\Delta_k \sim (b - ax_k)\widetilde{N}\left(\frac{1}{a}, \sigma, \frac{1}{a}(1 \pm \varepsilon)\right)$

Theorem

Let $x_0 = 0$, $x_{k+1} = x_k + \Delta_k$ where Δ_k is the random variable distributed as $(b - ax_k)\widetilde{N}\left(\frac{1}{a}, \sigma, \frac{1}{a}(1 \pm \varepsilon)\right)$ where $a, \varepsilon, \sigma > 0, b \in \mathbb{R}$. Then if $\varepsilon \leqslant e$ then $x_k \xrightarrow{P} \frac{b}{a}$. If $\varepsilon > e$ and $F(\varepsilon, a\sigma) < 0$ where

$$F(\varepsilon, a\sigma) = \log\left(\sqrt{2}a\sigma\right) + \left(\int_0^{\frac{\varepsilon}{\sqrt{2}a\sigma}} e^{-x^2}\, dx\right)^{-1} \left(\int_0^{\frac{\varepsilon}{\sqrt{2}a\sigma}} e^{-x^2} \log x\, dx\right),$$

then $x_k \xrightarrow{P} \frac{b}{a}$.

Remark

If $\varepsilon \to \infty$ then the first integral $\to \frac{\sqrt{\pi}}{2}$, the second one $\to -\frac{\sqrt{\pi}}{4}(\gamma + 2\log 2)$, so $F(\varepsilon, a\sigma) \to \log\frac{a\sigma}{\sqrt{2}} - \frac{\gamma}{2} < 0 \Rightarrow a\sigma < \sqrt{2}e^{\gamma/2}$

For an equation

$$ax + by = c$$

We have the distribution of solutions

$$P((x, y)) \propto e^{-\beta(ax+by-c)^2}$$

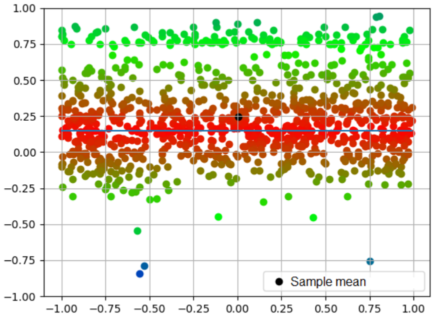
- If we want to find the limit distribution of solutions then we cannot impose no restrictions on the values of solutions since the integral $\iint_{\mathbb{R}^2} e^{-\beta(ax+by-c)^2} dxdy$ does not converge.
- If we let Ω be the set of values that solutions can take then the limit distribution has the density function

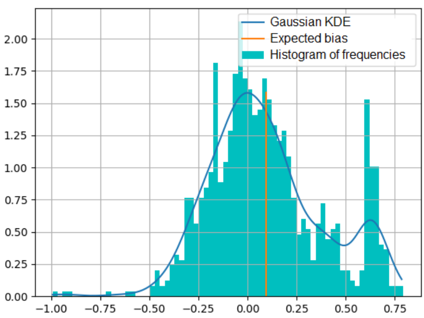
$$\frac{e^{-\beta(ax+by-c)^2}}{\iint\limits_{\Omega} e^{-\beta(ax+by-c)^2} dxdy} \cdot \mathbf{1}_{\Omega}(x, y)$$

An equation with two variables

Limit distribution of solutions

- We take $\Omega = [-1,1]^2$ and sample 1000 times the «solutions» of the equations $2y = 0.3$ with precision $R = 8$ bits.
- Also we project samples onto the line orthogonal to $2y = 0.3$.
- Expected bias is the mean distance between samples and the line $2y = 0.3$.

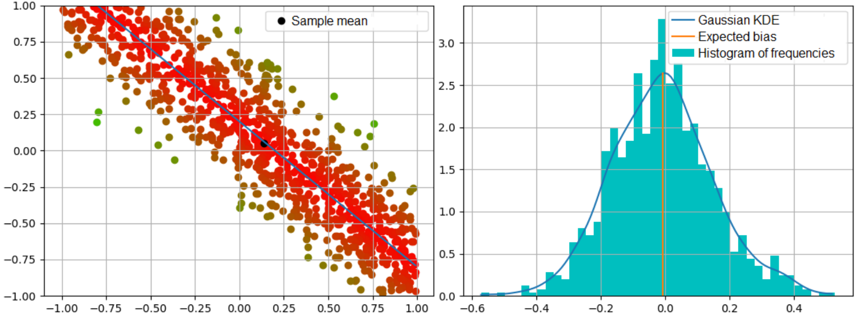




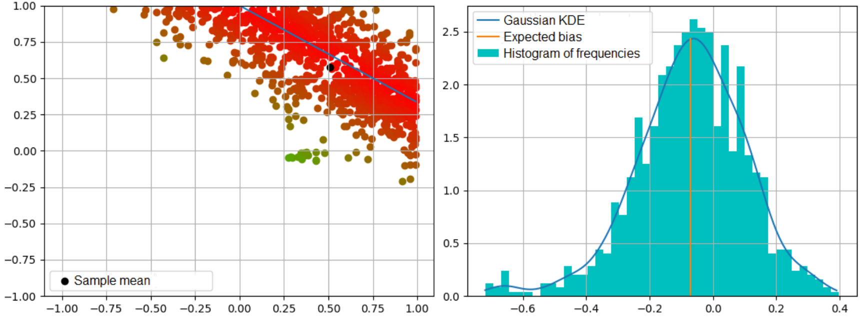
An equation with two variables

Limit distribution of solutions

Samples for $x + y = 0.2$.



Samples for $2x + 3y = 3$.



Two equations with one variable

$$\begin{cases} a_1 x = b_1, \\ a_2 x = b_2. \end{cases}$$

- Solving this system is equivalent to solving one equation

$$||a||x = \left(\frac{a}{||a||}, b \right),$$

  whose solution is pseudo-solution of minimal norm of the above system. Here $a = (a_1, a_2),\ b = (b_1, b_2)$.
- This can be generalized to any overdeterminated system, i.e. finding a normal pseudo-solution of the system $(n + k) \times n$ is equivalent to solving some system $n \times n$.
- But is there an efficient algorithm for finding this quadratic system?

$$Ax = b \quad \text{or} \quad \begin{cases} a_{11}x_1 + a_{12}x_2 = b_1, \\ a_{21}x_1 + a_{22}x_2 = b_2. \end{cases}$$

- Let the Boltzmann distribution of solutions have the Hamiltonian $||Ax - b||^2$ and parameter β.
- Let $\det A \neq 0$, A_1 and A_2 be the first and the second columns of A. If there is no restrictions on the range of values of x
- then the limit distribution of solutions is $\mathcal{N}(\mu, \mathcal{K})$, where

$$\mu = A^{-1}b, \quad \mathcal{K}^{-1} = 2\beta \begin{pmatrix} (A_1, A_1) & (A_1, A_2) \\ (A_1, A_2) & (A_2, A_2) \end{pmatrix}$$

Sampling from «almost» normal distribution using AQC

- For the one dimensional case if we want to sample from normal distribution $\mathcal{N}(\mu, \sigma)$ then we can construct a Hamiltonian for the Boltzmann distribution with parameter β.

$$H(x) = \left(\frac{x}{\sigma\sqrt{2\beta}} - \frac{\mu}{\sigma\sqrt{2\beta}} \right)^2$$

  where we used the statement about the limit distribution of solutions of an equation $ax = b$.
- The same we can do for multivariate normal distribution.
- But it is time-consuming to construct a Hamiltonian because in order to do this we (again) need to invert given covariance matrix.