Preconditioned Conjugate Gradient Method.

$$Q\vec{x} = \vec{b}$$

$$M^{-1}Q\vec{x} = M^{-1}\vec{b}$$

$$\underbrace{M^{-\frac{1}{2}}QM^{-\frac{1}{2}}}_{\breve{Q}}\ \underbrace{M^{\frac{1}{2}}\vec{x}}_{\breve{x}} = \underbrace{M^{-\frac{1}{2}}\vec{b}}_{\breve{b}}$$

① $M^{\frac{1}{2}}\vec{x} = \breve{x}$

② $M^{-\frac{1}{2}}\vec{b} = \breve{b}$

③ $M^{-\frac{1}{2}}QM^{-\frac{1}{2}} = \breve{Q}$

Apply cg to: $\breve{Q}\breve{x} = \breve{b}$

$$\breve{d}_0 = -\hat{g}_0 = \breve{b} - \breve{Q}\breve{x}_0$$

$$\Leftrightarrow \quad \breve{d}_0 = -\breve{g}_0 = M^{-\frac{1}{2}}\vec{b} - M^{-\frac{1}{2}}QM^{-\frac{1}{2}}M^{\frac{1}{2}}\vec{x}$$

$$\Leftrightarrow \quad M^{\frac{1}{2}}\breve{d}_0 = -M^{\frac{1}{2}}\breve{g}_0 = \vec{b} - Q\vec{x}$$

④ $M^{\frac{1}{2}}\breve{d}_0 = \vec{d}_0 \quad \Rightarrow \quad \breve{d}_k = M^{-\frac{1}{2}}\vec{d}_k$

⑤ $M^{\frac{1}{2}}\breve{g}_0 = \vec{g}_0 \quad \Rightarrow \quad \breve{g}_k = M^{-\frac{1}{2}}\vec{g}_k \quad \Rightarrow \quad \vec{d}_0 = \vec{g}_0 = \vec{b} - Q\vec{x}_0$ ⓐ

$$\breve{x}_{k+1} = \breve{x}_k + \breve{\alpha}_k\breve{d}_k$$

$$M^{\frac{1}{2}}\vec{x}_{k+1} = M^{\frac{1}{2}}\vec{x}_k + \breve{\alpha}_k M^{-\frac{1}{2}}\vec{d}_k$$

$$\vec{x}_{k+1} = \vec{x}_k + \breve{\alpha}_k M^{-1}\vec{d}_k$$

⑥ $M^{-1}\vec{d}_k = \vec{p}_k$

$$\Rightarrow \quad \vec{x}_{k+1} = \vec{x}_k + \breve{\alpha}_k\vec{p}_k \quad ⓑ$$

$$M^{-\frac{1}{2}}\vec{g}_{k+1} = \breve{g}_{k+1} = \breve{Q}\breve{x}_{k+1} - \breve{b}$$

$$= M^{-\frac{1}{2}}QM^{-\frac{1}{2}}M^{\frac{1}{2}}\vec{x}_{k+1} - M^{-\frac{1}{2}}\vec{b} \quad \Rightarrow \quad \vec{g}_{k+1} = Q\vec{x}_{k+1} - \vec{b}$$

$$\Rightarrow \quad \vec{g}_{k+1} = Q(\vec{x}_k + \breve{\alpha}_k\vec{p}_k) - \vec{b} = \vec{g}_k + \breve{\alpha}_k Q\vec{p}_k \quad ⓒ$$

$$\hat{d}_{k+1} = -\hat{g}_{k+1} + \hat{\beta}_k \hat{d}_k$$

$$M^{-1/2} \vec{d}_{k+1} = -M^{-1/2} \vec{g}_{k+1} + \hat{\beta}_k M^{-1/2} \vec{d}_k$$

$$M^{-1} \vec{d}_{k+1} = -M^{-1} \vec{g}_{k+1} + \hat{\beta}_k M^{-1} \vec{d}_k$$

$$\vec{p}_{k+1} = -\vec{z}_{k+1} + \hat{\beta}_k \vec{p}_k \quad \text{(d)}$$

(7) $\vec{z}_k := M^{-1} \vec{g}_k \iff M \vec{z}_k = \vec{g}_k$

$$\hat{\alpha}_k = \frac{\hat{g}_k^* \hat{g}_k}{\hat{d}_k^* \hat{Q} \hat{d}_k} = \frac{\vec{g}_k^* M^{-1/2} M^{-1/2} \vec{g}_k}{\vec{d}_k^* M^{-1/2} M^{-1/2} Q M^{-1/2} M^{-1/2} \vec{d}_k}$$

$$= \frac{\vec{g}_k^* M^{-1} \vec{g}_k}{\vec{d}_k^* M^{-1} Q M^{-1} \vec{d}_k} = \frac{\vec{g}_k^* \vec{z}_k}{\vec{p}_k^* Q \vec{p}_k} \quad \text{(e)}$$

$$\hat{\beta}_k = \frac{\hat{g}_{k+1}^* \hat{g}_{k+1}}{\hat{g}_k^* \hat{g}_k} = \frac{\vec{g}_{k+1}^* \vec{z}_{k+1}}{\vec{g}_k^* \vec{z}_k} \quad \text{(f)}$$

Preconditioned Conjugate Gradient Method.

Initialization: $\vec{g}_0 \overset{(a)}{=} \vec{b} - Q\vec{x}_0$

Solve $M\vec{z}_0 \overset{(7)}{=} \vec{g}_0$, $\vec{p}_0 \overset{(7)}{=} \vec{z}_0$

(i) $\vec{x}_{k+1} \overset{(b)}{=} \vec{x}_k + \hat{\alpha}_k \vec{p}_k$

$$\hat{\alpha}_k \overset{(e)}{=} \frac{\vec{g}_k^* \vec{z}_k}{\vec{p}_k^* Q \vec{p}_k}$$

(ii) $\vec{g}_{k+1} \overset{(c)}{=} \vec{g}_k + \hat{\alpha}_k Q \vec{p}_k$

(iii) Solve $M\vec{z}_{k+1} \overset{(7)}{=} \vec{g}_{k+1}$

(iv) $\vec{p}_{k+1} \overset{(d)}{=} -\vec{z}_{k+1} + \hat{\beta}_k \vec{p}_k$

where $\hat{\beta}_k \overset{(f)}{=} \dfrac{\vec{g}_{k+1}^* \vec{z}_{k+1}}{\vec{g}_k^* \vec{z}_k}$

Note that it requires one matrix vector multiplication $A \cdot p_k$, and one matrix solution $M \cdot \vec{z}_k = \vec{p}_k$ in each iteration