more on

Conjugate Gradients
Diagonalization

Conjugate Gradients Diagonalization

- For each band, given a trial eigenpair: $\{|\phi_i^{(n)}\rangle, \varepsilon_i\}$
- Minimize the single particle energy

$$E(|\phi_i\rangle) = \langle\phi_i|H_{KS}|\phi_j\rangle$$

by (pre-conditioned) CG method

subject to the constraints

$$\langle\phi_i|S|\phi_j\rangle = \delta_{ij}, \quad \forall j \leq i$$

- Repeat for next band until completed

Steepest Descent Minimization

$$f(x) = \frac{1}{2} x A x - b x$$

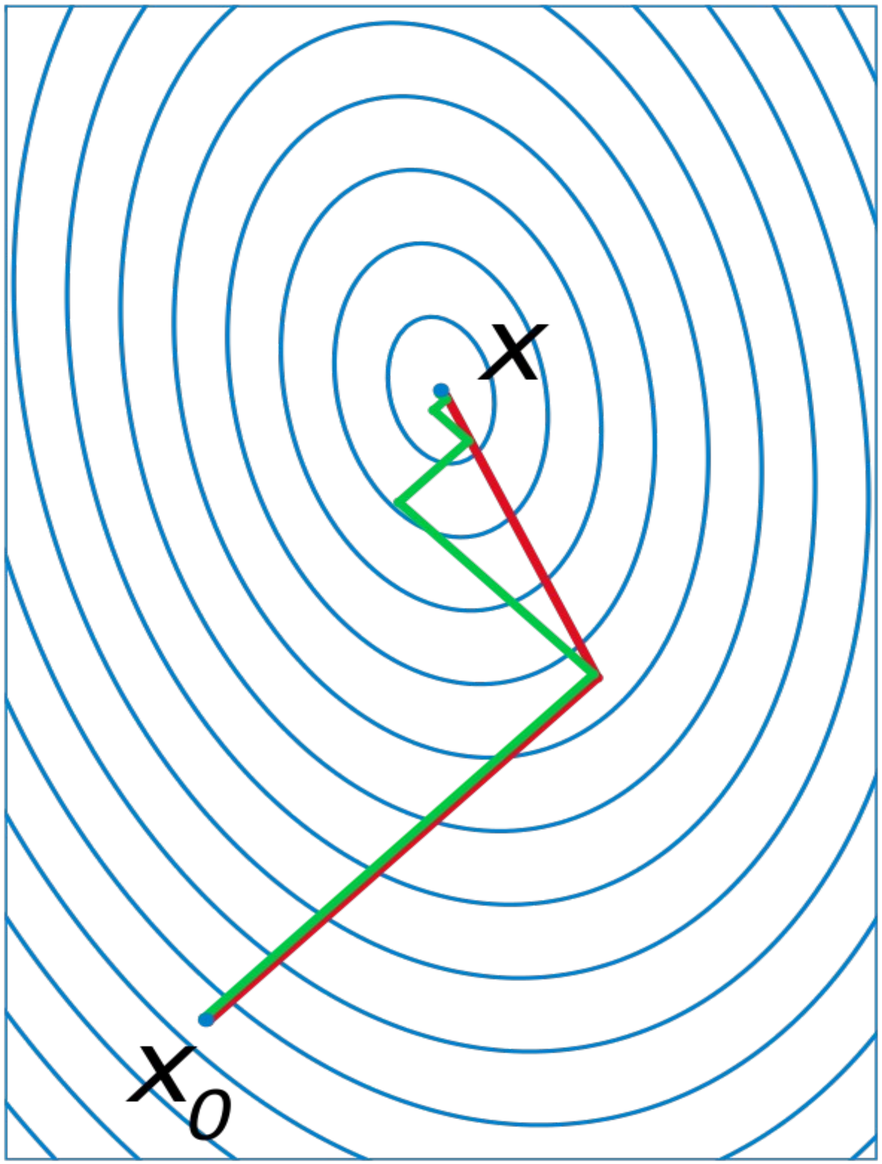
$$g(x) = -\nabla f(x) = b - Ax$$

$$x = x_0 \qquad g_0 = b - A x_0$$

$$x_{k+1} = x_k + \lambda g_k$$
$$g_{k+1} = g_k - \lambda A g_k$$
$$\lambda = \frac{g_k g_k}{g_k A g_k}$$

subsequent minimizations
are orthogonal !

keep updating the same
directions !



Conjugate Gradients Minimization

$$f(x) = \frac{1}{2} x A x - b x \qquad g(x) = -\nabla f(x) = b - Ax$$

$$x = x_0 + \sum_k \alpha_k h_k \qquad g_0 = b - Ax_0$$

$$f(x) = f(x_0) + \frac{1}{2} \sum_{kl} \alpha_k \; h_k A h_l \; \alpha_l - \sum_k g_0 h_k \; \alpha_k$$

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$$f(x) = f(x_0) + \frac{1}{2} \sum_{kl} \alpha_k \, h_k A h_l \, \alpha_l - \sum_k g_0 h_k \, \alpha_k$$

If conjugate directions are considered: $h_k A h_l = 0$ for $k \neq l$

$$f(x) = f(x_0) + \frac{1}{2} \sum_{k} \alpha_k^2 \, h_k A h_k - \sum_k g_0 h_k \, \alpha_k$$

each term add to the solution w/o spoiling previous steps.
after N steps the minimization terminates at the minimum.

Conjugate Gradients Minimization

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$$x_0, g_0, h_0 = g_0$$

$$x_{k+1} = x_k + \alpha_k h_k \qquad \alpha_k = \frac{g_0 h_k}{h_k A h_k}$$

$$g_{k+1} = g_k - \alpha_k A h_k$$

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$$g_{k+1} = g_k - \alpha_k A h_k$$

because $h_l A h_k = 0, \quad \forall l < k$

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because $h_l A h_k = 0, \quad \forall l < k$

$$h_{k+1} = g_{k+1} + \beta_k h_k$$

$$h_{k+1} A h_k = 0 \quad \Longrightarrow \quad \beta_k = -\frac{h_k A g_{k+1}}{h_k A h_k}$$

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$$g_{k+1} = g_k - \alpha_k A h_k$$

because $g_k h_{k-1} = 0$

$$h_{k+1} = g_{k+1} + \beta_k h_k$$

$$h_{k+1} A h_k = 0 \implies \beta_k = -\frac{h_k A g_{k+1}}{h_k A h_k}$$

Conjugate Gradients Minimization

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because $g_k h_{k-1} = 0$

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$$h_{k+1} A h_k = 0 \quad \Longrightarrow \quad \beta_k = -\frac{h_k A g_{k+1}}{h_k A h_k} = \frac{g_{k+1} g_{k+1}}{g_k g_k}$$

because $g_{k+1} g_k = 0$

Conjugate Gradients Minimization

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$$x_{k+1} = x_k + \alpha_k h_k$$

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$$\boxed{\alpha_k =} \frac{g_0 h_k}{h_k A h_k} = \frac{g_k h_k}{h_k A h_k} = \boxed{\frac{g_k g_k}{h_k A h_k}}$$

because $\quad g_k h_{k-1} = 0$

$$h_{k+1} = g_{k+1} + \beta_k h_k$$

$$h_{k+1} A h_k = 0 \quad \Longrightarrow \quad \boxed{\beta_k =} - \frac{h_k A g_{k+1}}{h_k A h_k} = \boxed{\frac{g_{k+1} g_{k+1}}{g_k g_k}}$$

Conjugate Gradients Minimization

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Conjugate Gradients Minimization (general)

$$f(x) \approx \frac{1}{2} x A x - b x \qquad g(x) = -\nabla f(x)$$

$$x = x_0 + \sum_k \alpha_k h_k \qquad g_0 = -\nabla f(x_0)$$

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$$x_0, g_0, h_0 = g_0$$

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$$x_0, g_0, h_0 = g_0$$

$$x_{k+1} = x_k + \alpha_k h_k \qquad \cancel{\alpha_k = \frac{g_k g_k}{h_k A h_k}}$$

replaced with line minim

$$g_{k+1} = g_k - \alpha_k A h_k$$

$$\beta_k = \frac{g_{k+1} g_{k+1}}{g_k g_k}$$

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$$x_0, g_0, h_0 = g_0$$

$$\cancel{\alpha_k = \frac{g_k g_k}{h_k A h_k}}$$ replaced with line minim.

$$x_{k+1} = x_k + \alpha_k h_k$$

$$g_{k+1} = \cancel{g_k - \alpha_k A h_k} = -\nabla f(x_k)$$ gradient at the minimum

$$\beta_k = \frac{g_{k+1} g_{k+1}}{g_k g_k}$$

$$h_{k+1} = g_{k+1} + \beta_k h_k$$

Conjugate Gradients Minimization (general)

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replaced with line minim.

$$g_{k+1} = \cancel{g_k - \alpha_k A h_k} = -\nabla f(x_k)$$

gradient at the minimum

$$\beta_k = \frac{g_{k+1} g_{k+1}}{g_k g_k} = \frac{(g_{k+1} - g_k) g_{k+1}}{g_k g_k}$$

$$h_{k+1} = g_{k+1} + \beta_k h_k$$

Fletcher-Reeves

Polak-Ribiere

Conjugate Gradients Diagonalization

- For each band, given a trial eigenpair: $\{|\phi_i^{(n)}\rangle, \varepsilon_i\}$

- Minimize the single particle energy

$$E(|\phi_i\rangle) = \langle\phi_i|H_{KS}|\phi_j\rangle$$

by (pre-conditioned) CG method

subject to the constraints

$$\langle\phi_i|S|\phi_j\rangle = \delta_{ij}, \quad \forall j \leq i$$

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Preconditioned Conjugate Gradients Minimization

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If conjugate directions are considered: $h_k A h_l = 0$ for $k \neq l$

The method is guaranteed to converge after N steps.

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The method is guaranteed to converge after N steps.

Not very appealing if N is very large.

Preconditioned Conjugate Gradients Minimization

$$f(x) = \frac{1}{2} xAx - bx \qquad\qquad g(x) = -\nabla f(x) = b - Ax$$

Define $x = Py$ such that $PAP \approx const$

Apply the algorithm to the transformed problem

Preconditioned Conjugate Gradients Minimization

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Apply the algorithm to the transformed problem

$$y_0, \;\; \tilde{g}_0 = P(b - APy_0), \;\; \tilde{h}_0 = \tilde{g}_0$$

$$\alpha_k = \frac{\tilde{g}_k \tilde{g}_k}{\tilde{h}_k PAP \tilde{h}_k}$$

$$y_{k+1} = y_k + \alpha_k \tilde{h}_k$$

$$\tilde{g}_{k+1} = \tilde{g}_k - \alpha_k PAP \tilde{h}_k$$

$$\beta_k = \frac{\tilde{g}_{k+1} \tilde{g}_{k+1}}{\tilde{g}_k \tilde{g}_k}$$

$$\tilde{h}_{k+1} = \tilde{g}_{k+1} + \beta_k \tilde{h}_k$$

Preconditioned Conjugate Gradients Minimization

$$f(x) = \frac{1}{2} x A x - b x \qquad\qquad g(x) = -\nabla f(x) = b - A x$$

Define $x = P y$ such that $PAP \approx const$

$$x_k = P y_k, \quad h_k = P \tilde{h}_k, \quad g_k = P \tilde{g}_k$$

Apply the algorithm to the transformed problem

$$x_0, \;\; g_0 = P^2 (b - A x_0), \;\; h_0 = g_0$$

$$\alpha_k = \frac{g_k P^{-2} g_k}{h_k A h_k}$$

$$x_{k+1} = x_k + \alpha_k h_k$$

$$g_{k+1} = g_k - \alpha_k P^2 A h_k$$

$$\beta_k = \frac{g_{k+1} P^{-2} g_{k+1}}{g_k P^{-2} g_k}$$

$$h_{k+1} = g_{k+1} + \beta_k h_k$$