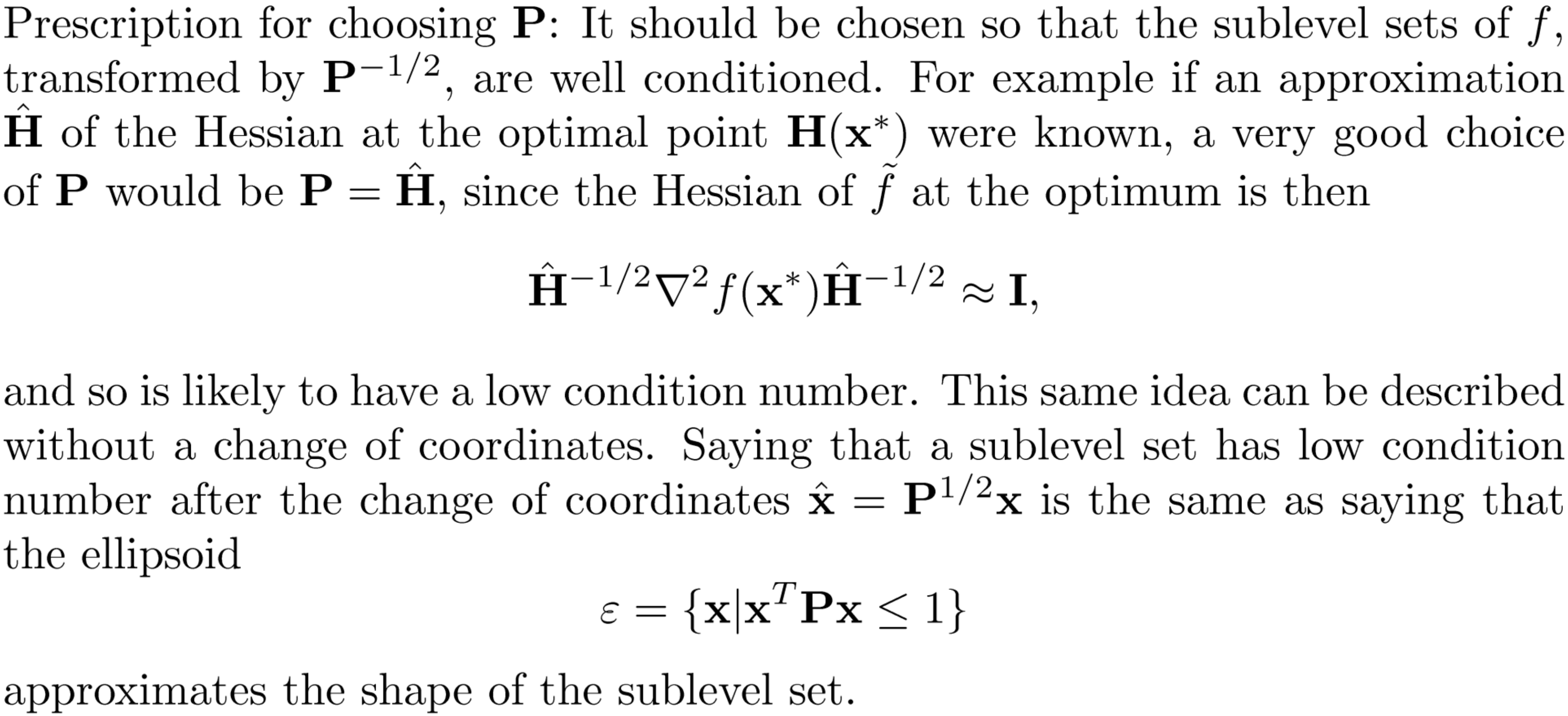
# Descent methods

- Choice of norm for steepest descent



Prescription for choosing $\mathbf{P}$: It should be chosen so that the sublevel sets of $f$, transformed by $\mathbf{P}^{-1/2}$, are well conditioned. For example if an approximation $\hat{\mathbf{H}}$ of the Hessian at the optimal point $\mathbf{H}(\mathbf{x}^*)$ were known, a very good choice of $\mathbf{P}$ would be $\mathbf{P} = \hat{\mathbf{H}}$, since the Hessian of $\tilde{f}$ at the optimum is then

$$\hat{\mathbf{H}}^{-1/2}\nabla^2 f(\mathbf{x}^*)\hat{\mathbf{H}}^{-1/2} \approx \mathbf{I},$$

and so is likely to have a low condition number. This same idea can be described without a change of coordinates. Saying that a sublevel set has low condition number after the change of coordinates $\hat{\mathbf{x}} = \mathbf{P}^{1/2}\mathbf{x}$ is the same as saying that the ellipsoid

$$\varepsilon = \{\mathbf{x} | \mathbf{x}^T\mathbf{P}\mathbf{x} \leq 1\}$$

approximates the shape of the sublevel set.

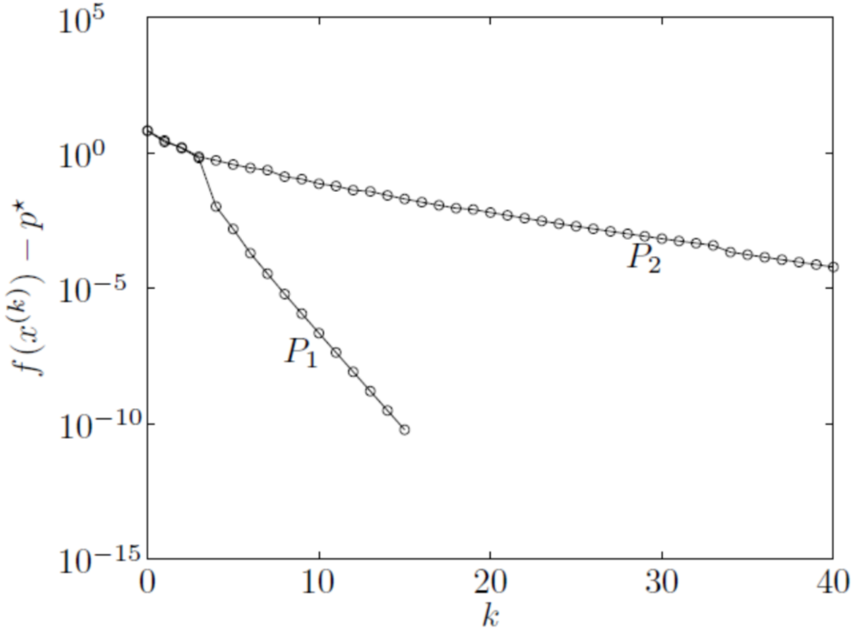
# Descent methods

- Examples

$$f(x_1, x_2) = e^{x_1+3x_2-0.1} + e^{x_1-3x_2-0.1} + e^{-x_1-0.1}.$$

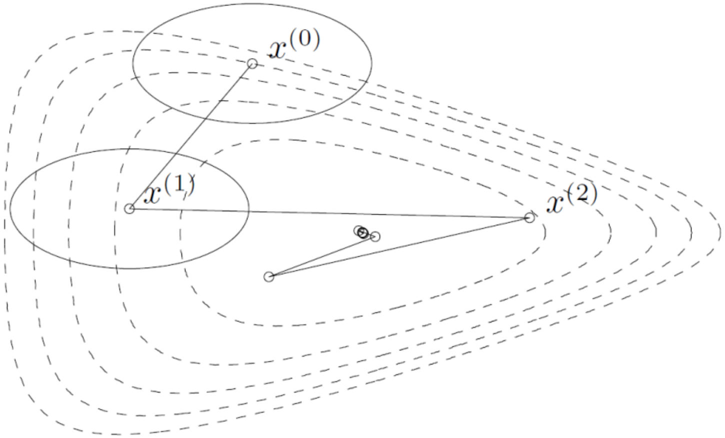
$$\mathbf{P}_1 = \begin{bmatrix} 2 & 0 \\ 0 & 8 \end{bmatrix}, \mathbf{P}_2 = \begin{bmatrix} 8 & 0 \\ 0 & 2 \end{bmatrix}.$$

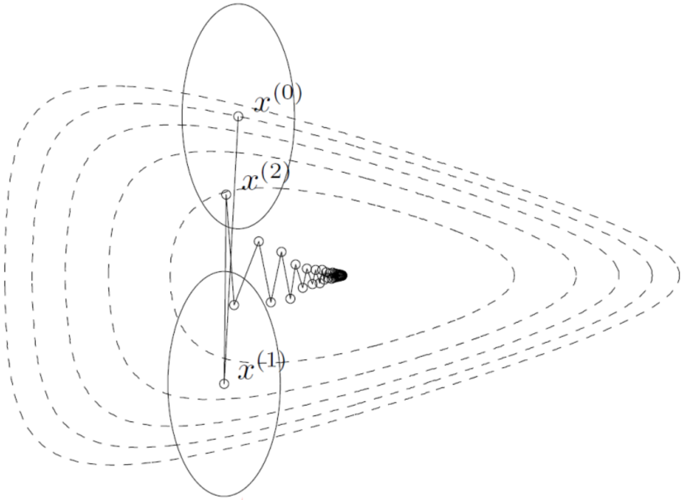
In both cases we use a backtracking line search with $\alpha = 0.1$ and $\beta = 0.7$.

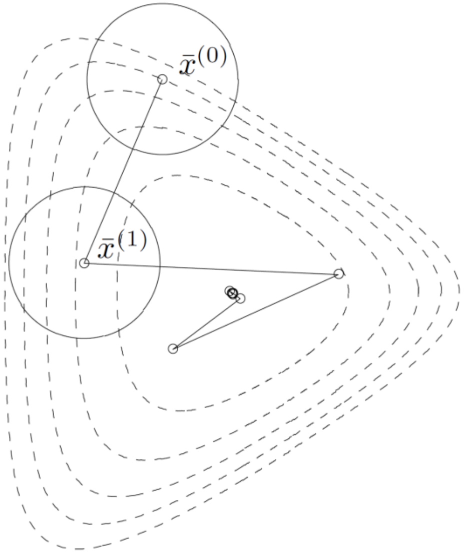


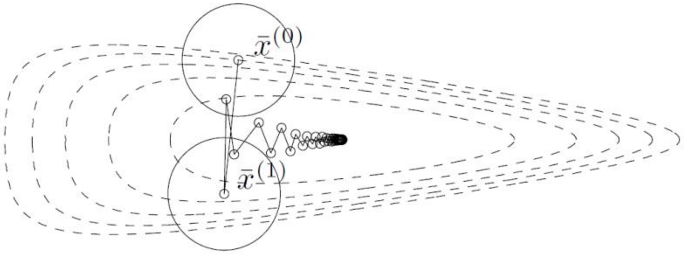
# Descent methods

- Examples









# Newton's method

$$f(\mathbf{x}) \approx f(\mathbf{x}^{(k)}) + \mathbf{g}^{(k)T}(\mathbf{x}-\mathbf{x}^{(k)}) + \frac{1}{2}(\mathbf{x}-\mathbf{x}^{(k)})^T F(\mathbf{x}^{(k)})(\mathbf{x}-\mathbf{x}^{(k)}) \triangleq q(\mathbf{x}),$$

where, for simplicity, we use the notation $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)})$. Applying the First-Order Necessary Condition (FONC) to $q$ yields

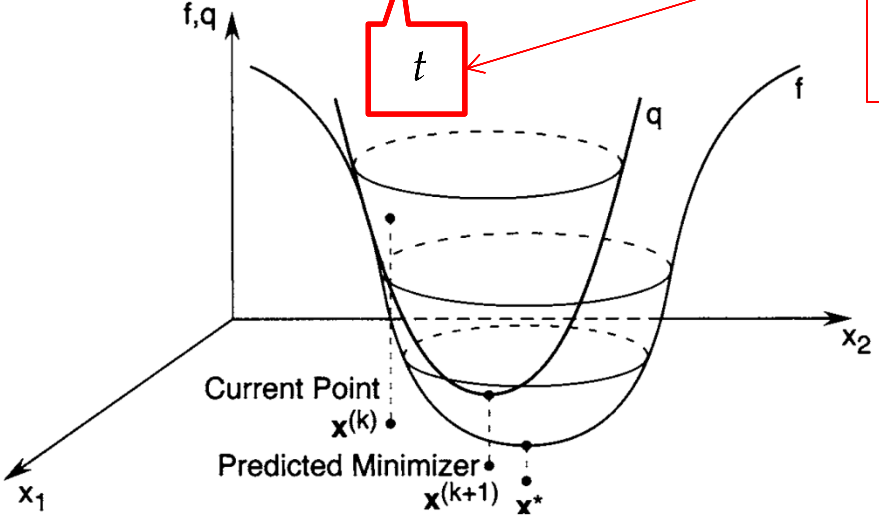
$$\mathbf{0} = \nabla q(\mathbf{x}) = \mathbf{g}^{(k)} + \mathbf{F}(\mathbf{x}^{(k)})(\mathbf{x}-\mathbf{x}^{(k)}).$$

If $\mathbf{F}(\mathbf{x}^{(k)}) \succ \mathbf{0}$, then $q$ achieves a minimum at

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mathbf{F}(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)}.$$

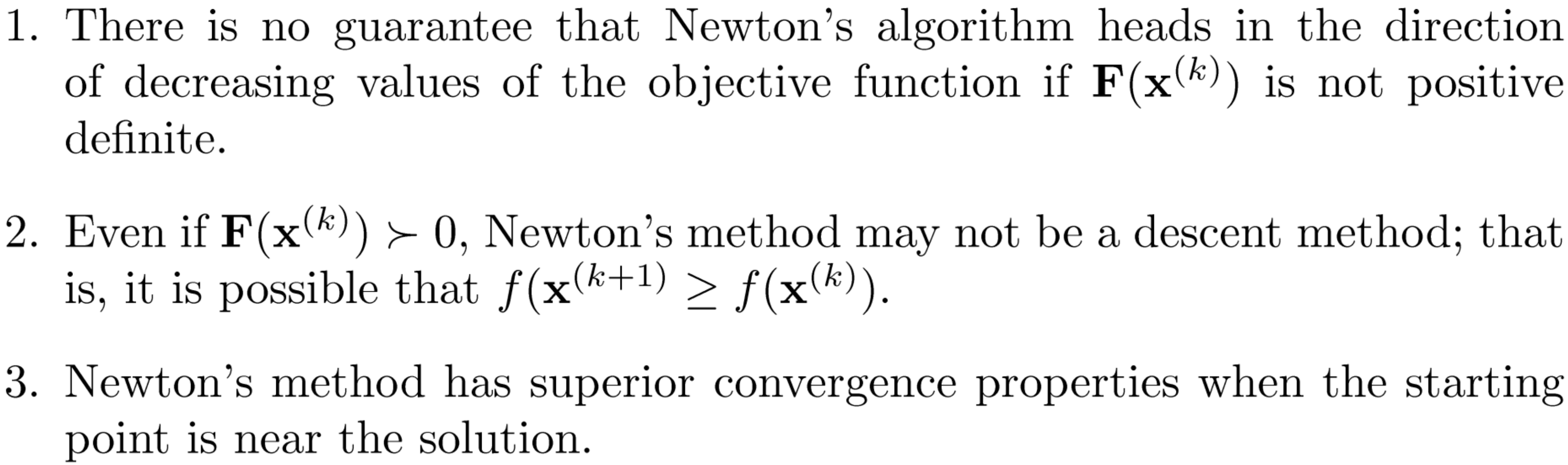
$t$

different from Boyd's book, which is called *damped Newton method*



# Newton's Method

- Analysis of Newton's Method



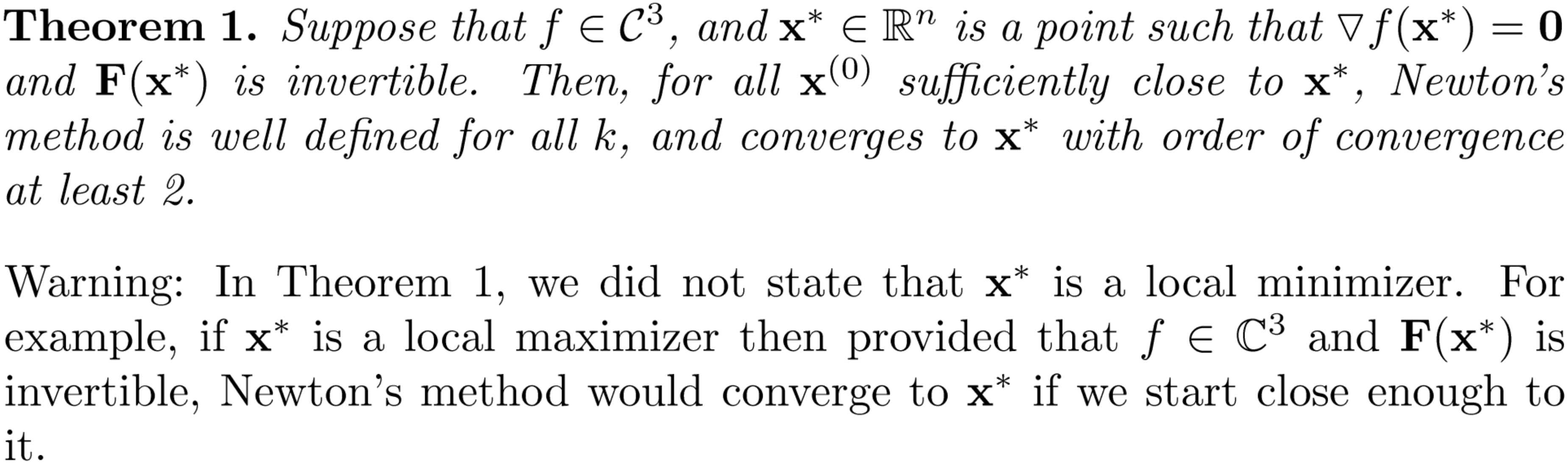
1. There is no guarantee that Newton's algorithm heads in the direction of decreasing values of the objective function if $\mathbf{F}(\mathbf{x}^{(k)})$ is not positive definite.

2. Even if $\mathbf{F}(\mathbf{x}^{(k)}) \succ 0$, Newton's method may not be a descent method; that is, it is possible that $f(\mathbf{x}^{(k+1)} \geq f(\mathbf{x}^{(k)})$.

3. Newton's method has superior convergence properties when the starting point is near the solution.

# Newton's Method

- Analysis of Newton's Method



**Theorem 1.** *Suppose that $f \in \mathcal{C}^3$, and $\mathbf{x}^* \in \mathbb{R}^n$ is a point such that $\nabla f(\mathbf{x}^*) = \mathbf{0}$ and $\mathbf{F}(\mathbf{x}^*)$ is invertible. Then, for all $\mathbf{x}^{(0)}$ sufficiently close to $\mathbf{x}^*$, Newton's method is well defined for all $k$, and converges to $\mathbf{x}^*$ with order of convergence at least 2.*

Warning: In Theorem 1, we did not state that $\mathbf{x}^*$ is a local minimizer. For example, if $\mathbf{x}^*$ is a local maximizer then provided that $f \in \mathbb{C}^3$ and $\mathbf{F}(\mathbf{x}^*)$ is invertible, Newton's method would converge to $\mathbf{x}^*$ if we start close enough to it.

# Newton's Method

- Analysis of Newton's Method

**Theorem 2.** *Suppose that $f \in \mathcal{C}^2$ is strongly convex, with Lipschitz continuous second order derivative:*

$$\nabla^2 f(\mathbf{x}) \succeq m\mathbf{I}, \quad \|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\|_F \leq L\|\mathbf{x} - \mathbf{y}\|_2,$$

*and $\mathbf{x}^* \in \mathbb{R}^n$ is a local minimizer. Then, for all $\mathbf{x}^{(0)}$ sufficiently close to $\mathbf{x}^*$, Newton's method converges to $\mathbf{x}^*$ with order of convergence at least 2.*

$$\begin{aligned}
\|\nabla f(\mathbf{x}^+)\|_2 &= \|\nabla f(\mathbf{x} + \Delta\mathbf{x}_{nt}) - (\nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x})\Delta\mathbf{x}_{nt})\|_2 \\
&= \left\| \int_0^1 (\nabla^2 f(\mathbf{x} + t\Delta\mathbf{x}_{nt}) - \nabla^2 f(\mathbf{x}))\Delta\mathbf{x}_{nt} \mathrm{d}t \right\|_2 \\
&\leq \frac{L}{2}\|\Delta\mathbf{x}_{nt}\|_2^2 = \frac{L}{2}\|\nabla^2 f(\mathbf{x})^{-1}\nabla f(\mathbf{x})\|_2^2 \leq \frac{L}{2m^2}\|\nabla f(\mathbf{x})\|_2^2.
\end{aligned}$$

# Newton's Method

- Damped Newton's Method

**Theorem 3.** *Let* $\{\mathbf{x}^{(k)}\}$ *be the sequence generated by Newton's method for minimizing a given objective function* $f(\mathbf{x})$*. If the Hessian* $\mathbf{F}(\mathbf{x}^{(k)}) \succ \mathbf{0}$ *and* $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)}) \neq \mathbf{0}$*, then the direction*

$$\mathbf{d}^{(k)} = -\mathbf{F}(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)}$$

*from* $\mathbf{x}^{(k)}$ *to* $\mathbf{x}^{(k+1)}$ *is a descent direction for* $f$ *in the sense that*

$$\left\langle \mathbf{d}^{(k)}, \mathbf{g}^{(k)} \right\rangle < 0.$$

The above theorem motivates the following *Damped Newton's method*:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \mathbf{F}(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)},$$

where $\alpha_k$ is obtained by backtracking line search.

Note that $\alpha_k$ will eventually be chosen as 1.

# Newton's Method

- Damped Newton's Method

**Theorem 4.** *There are numbers* $\eta \in (0, m^2/L]$ *and* $\gamma > 0$ *such that:*

- *If* $\|\nabla f(\mathbf{x}^{(k)})\|_2 \geq \eta$, *then*

$$f(\mathbf{x}^{(k+1)}) - f(\mathbf{x}^{(k)}) \leq -\gamma.$$

- *If* $\|\nabla f(\mathbf{x}^{(k)})\|_2 < \eta$, *then the backtracking line search selects* $\alpha^{(k)} = 1$ *and*

$$\frac{L}{2m^2}\|\nabla f(\mathbf{x}^{(k+1)})\|_2 \leq \left(\frac{L}{2m^2}\|\nabla f(\mathbf{x}^{(k)})\|_2\right)^2.$$

# Newton's Method

- Drawbacks of Newton's method

1. Evaluation of $\mathbf{F}(\mathbf{x}^{(k)})$ for large $n$ can be computationally expensive.
2. Solve the system of linear equations $\mathbf{F}(\mathbf{x}^{(k)})\mathbf{d}^{(k)} = -\mathbf{g}^{(k)}$ is also computationally expensive.
3. The Hessian matrix may not be positive definite.

# Newton's Method

- Levenberg-Marquardt modification

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k(\mathbf{F}(\mathbf{x}^{(k)}) + \mu_k \mathbf{I})^{-1}\mathbf{g}^{(k)},$$

It is actually locally minimizing

$$f(\mathbf{x}) + \frac{\mu_k}{2}\|\mathbf{x} - \mathbf{x}^{(k)}\|^2.$$

Pure Newton's method: $\mu_k \to 0$.
Pure gradient method with small step size: $\mu_k \to \infty$.
In practice, we may start with a small value of $\mu_k$, and then slowly increase it until we find that the iteration is descent, that is $f(\mathbf{x}^{(k+1)}) < f(\mathbf{x}^{(k)})$.

# Newton's Method

- Gauss-Newton method for nonlinear least-squares

$$\min_{\mathbf{x}} \sum_{i=1}^{m} (r_i(\mathbf{x}))^2,$$

where $r_i : \mathbb{R} \to \mathbb{R}, i = 1, \cdots, m$, are given functions. This particular problem is called a *nonlinear least-squares problem.*

# Newton's Method

- Gauss-Newton method for nonlinear least-squares

Defining $\mathbf{r} = [r_1, \cdots, r_m]^T$, we write the objective function as $f(\mathbf{x}) = \mathbf{r}(\mathbf{x})^T \mathbf{r}(\mathbf{x})$. Denote the Jacobian matrix of $\mathbf{r}$ by $\mathbf{J}(\mathbf{x})$, then

$$\nabla f(\mathbf{x}) = 2\mathbf{J}(\mathbf{x})^T \mathbf{r}(\mathbf{x}).$$

$$\begin{aligned}\nabla^2 f(\mathbf{x}) = 2\frac{\mathbf{J}^T\mathbf{r}}{\partial \mathbf{x}^T}(\mathbf{x}) &= 2\left(\mathbf{J}^T\mathbf{J} + \sum_{i=1}^{m} \frac{\frac{\partial r_i}{\partial \mathbf{x}}}{\partial \mathbf{x}^T} r_i\right)(\mathbf{x}) \\ &= 2\left(\mathbf{J}^T\mathbf{J} + \sum_{i=1}^{m} r_i \nabla^2 r_i\right)(\mathbf{x}) = 2\left(\mathbf{J}^T\mathbf{J} + \mathbf{S}\right)(\mathbf{x}),\end{aligned}$$

where $\mathbf{S} = \sum_{i=1}^{m} r_i \nabla^2 r_i$. Therefore, Newton's method is given by

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - (\mathbf{J}(\mathbf{x})^T\mathbf{J}(\mathbf{x}) + \mathbf{S}(\mathbf{x}))^{-1}\mathbf{J}(\mathbf{x})^T\mathbf{r}(\mathbf{x}).$$

# Newton's Method

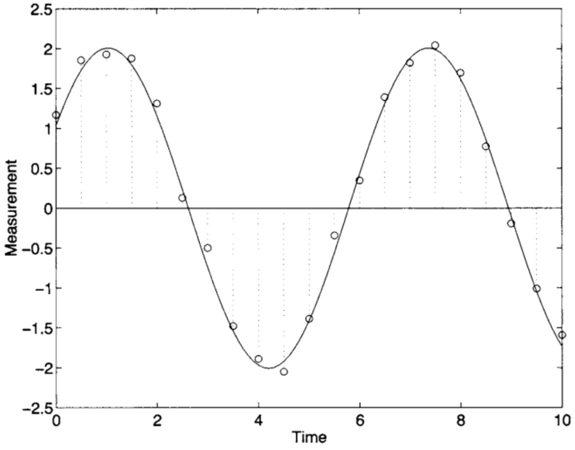
- Gauss-Newton method for nonlinear least-squares

Example: Suppose we are given $m$ measurements of a process at m points in time. Let $t_1, \cdots, t_m$ denote the measurement times, and $y_1, \cdots, y_m$ the measurement values. We wish to fit a sinusoid to the measurement data. The equation of the sinusoid is

$$y = A\sin(\omega\mathbf{x} + \phi)$$

with appropriate choices of the parameters $A, \omega$, and $\phi$. We construct the objective function

$$\sum_{i=1}^{m}(y_i - A\sin(\omega t_i + \phi))^2.$$

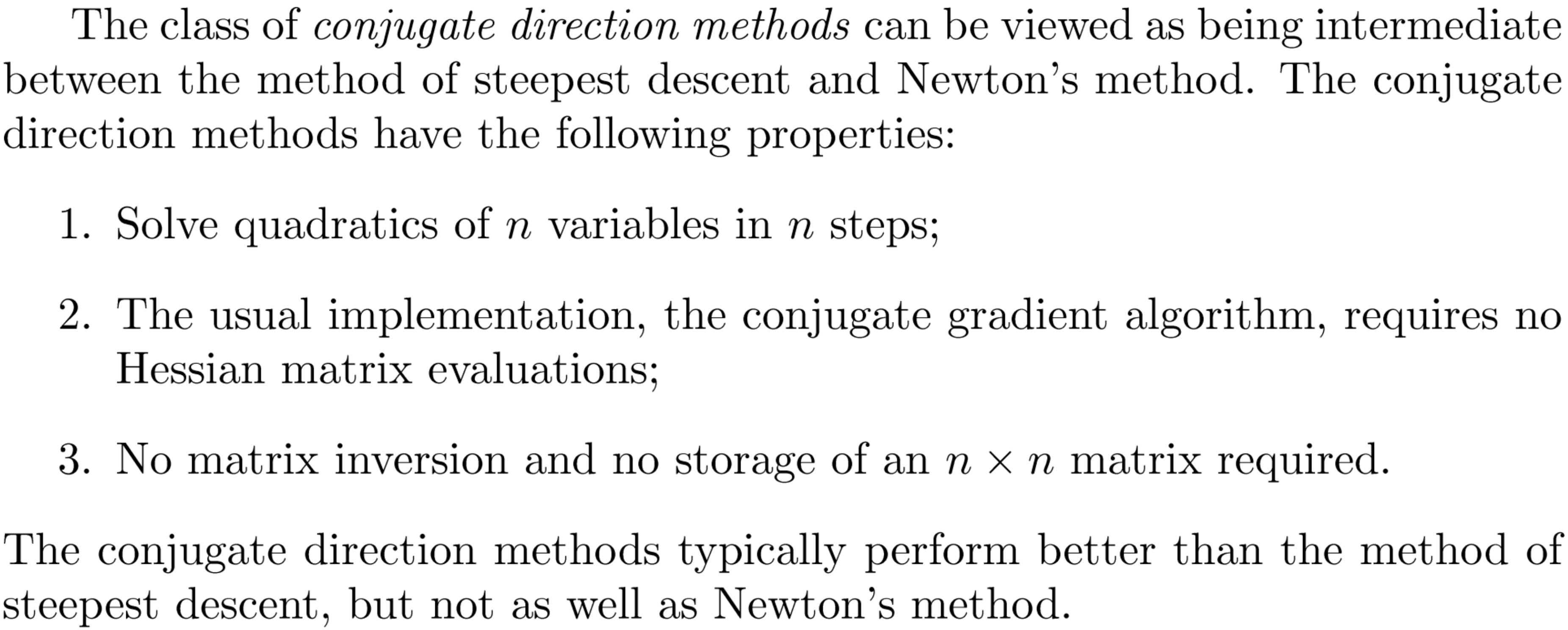


Let $\mathbf{x} = [A, \omega, \phi]^T$ represent the vector of decision variables. We therefore obtain a nonlinear least-squares problem with

$$r_i(\mathbf{x}) = y_i - A\sin(\omega t_i + \phi).$$

# Conjugate Direction Methods

- Introduction



The class of *conjugate direction methods* can be viewed as being intermediate between the method of steepest descent and Newton's method. The conjugate direction methods have the following properties:

1. Solve quadratics of $n$ variables in $n$ steps;

2. The usual implementation, the conjugate gradient algorithm, requires no Hessian matrix evaluations;

3. No matrix inversion and no storage of an $n \times n$ matrix required.

The conjugate direction methods typically perform better than the method of steepest descent, but not as well as Newton's method.

# Conjugate Direction Methods

- Introduction

**Definition 1.** *Let* $\mathbf{Q}$ *be a real symmetric* $n \times n$ *matrix. The directions* $\mathbf{d}^{(0)}, \mathbf{d}^{(1)}, \cdots, \mathbf{d}^{(m)}$ *are* $\mathbf{Q}$*-conjugate if, for all* $i \neq j$*, we have* $\mathbf{d}^{(i)T}\mathbf{Q}\mathbf{d}^{(j)} = 0$.

**Lemma 2.** *Let* $\mathbf{Q}$ *be a symmetric positive definite* $n \times n$ *matrix. If the directions* $\mathbf{d}^{(0)}, \mathbf{d}^{(1)}, \cdots, \mathbf{d}^{(k)} \in \mathbb{R}^n, k \leq n-1$*, are nonzero and* $\mathbf{Q}$*-conjugate, then they are linearly independent.*

$\mathbf{d}^{(0)}, \mathbf{d}^{(1)}, \cdots, \mathbf{d}^{(k)} \in \mathbb{R}^n, k \leq n-1$, are nonzero and $\mathbf{Q}$-conjugate iff $\{\tilde{\mathbf{d}}^{(i)}\}$ are mutually orthogonal, where $\tilde{\mathbf{d}}^{(i)} = \mathbf{Q}^{1/2}\mathbf{d}^{(i)}$.

# Conjugate Direction Methods

- The conjugate gradient algorithm for quadratic problems

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x} - \mathbf{x}^T\mathbf{b}, \mathbf{x} \in \mathbb{R}^n,$$

where $\mathbf{Q} = \mathbf{Q}^T \succ \mathbf{0}$. Our first search direction from an initial point $\mathbf{x}^{(0)}$ is in the direction of steepest descent; that is

$$\mathbf{d}^{(0)} = -\mathbf{g}^{(0)}.$$

Thus,

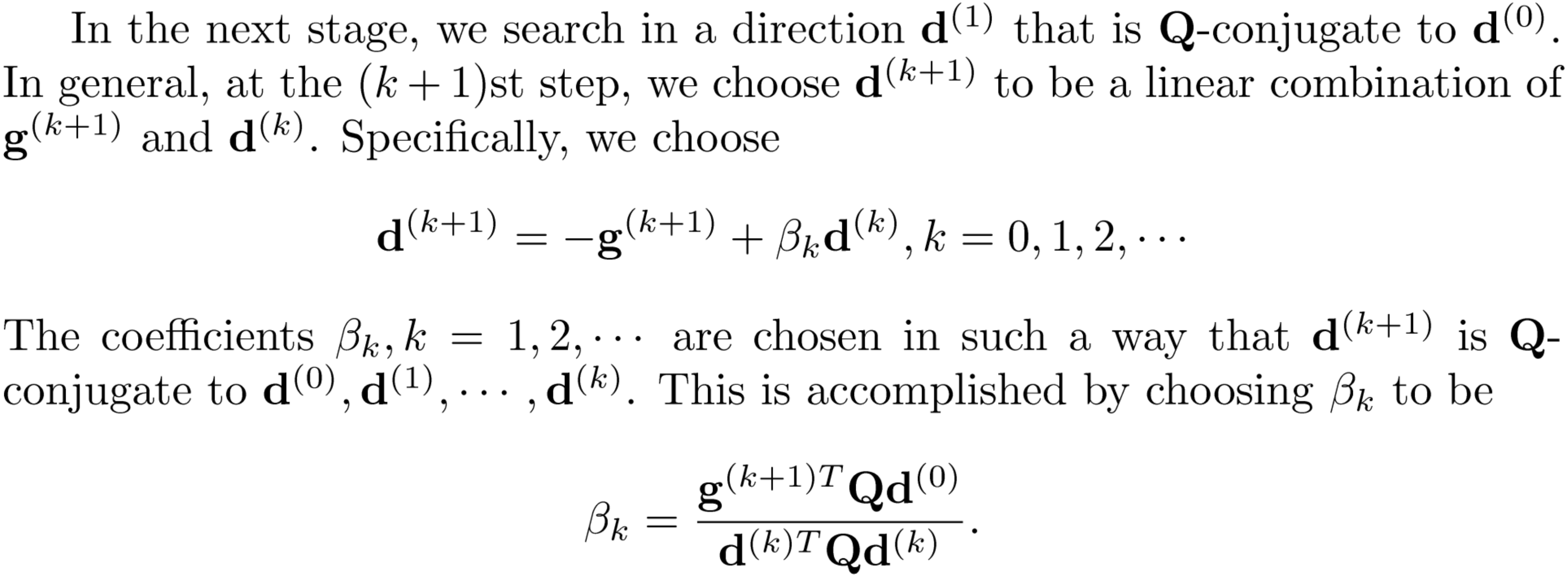
$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0\mathbf{d}^{(0)},$$

where

$$\alpha_0 = \arg\min_{\alpha>0} f(\mathbf{x}^{(0)} + \alpha\mathbf{d}^{(0)}) = -\frac{\mathbf{g}^{(0)T}\mathbf{d}^{(0)}}{\mathbf{d}^{(0)T}\mathbf{Q}\mathbf{d}^{(0)}}.$$

# Conjugate Direction Methods

- The conjugate gradient algorithm for quadratic problems



In the next stage, we search in a direction $\mathbf{d}^{(1)}$ that is $\mathbf{Q}$-conjugate to $\mathbf{d}^{(0)}$. In general, at the $(k+1)$st step, we choose $\mathbf{d}^{(k+1)}$ to be a linear combination of $\mathbf{g}^{(k+1)}$ and $\mathbf{d}^{(k)}$. Specifically, we choose

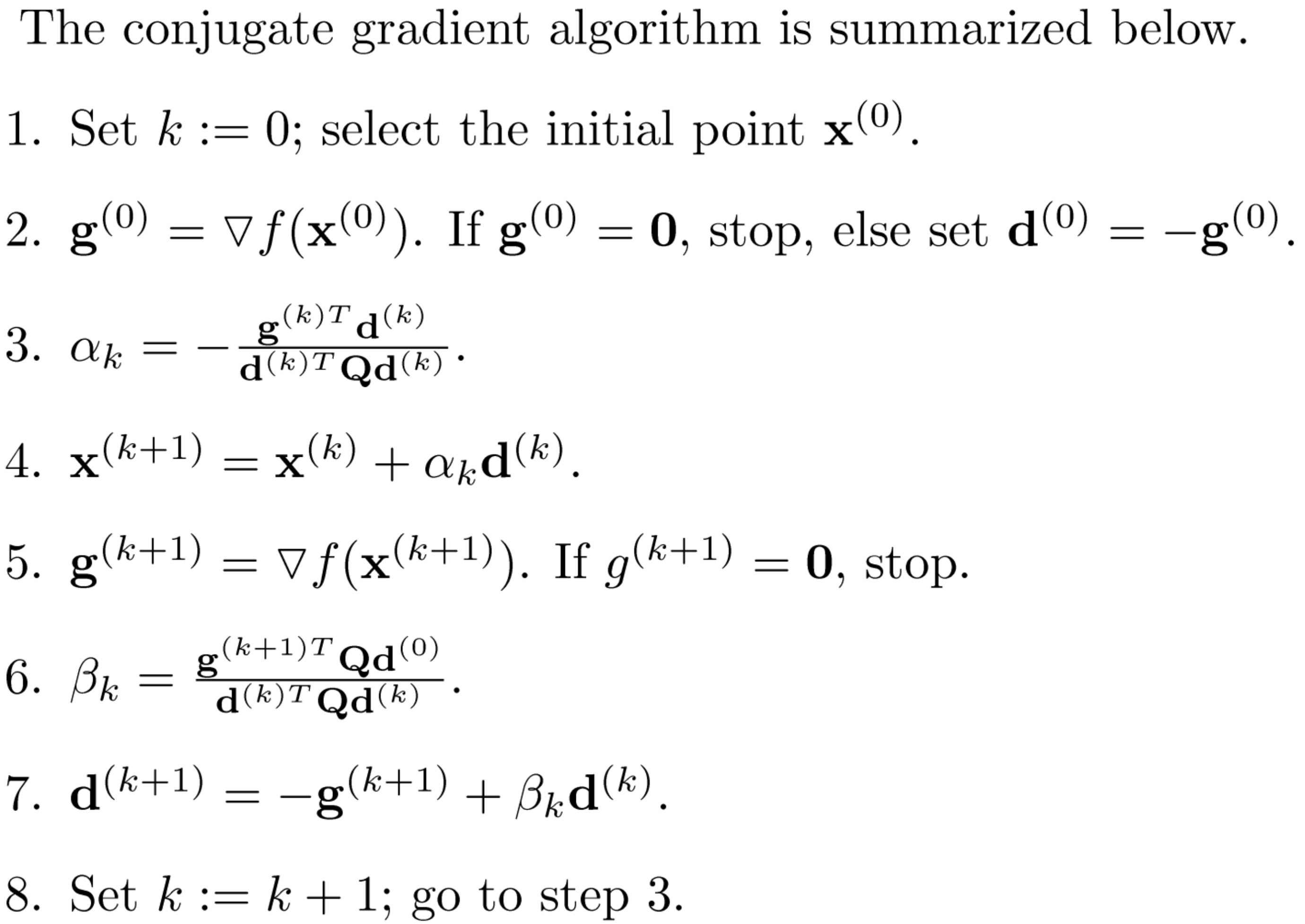
$$\mathbf{d}^{(k+1)} = -\mathbf{g}^{(k+1)} + \beta_k \mathbf{d}^{(k)}, k = 0, 1, 2, \cdots$$

The coefficients $\beta_k, k = 1, 2, \cdots$ are chosen in such a way that $\mathbf{d}^{(k+1)}$ is $\mathbf{Q}$-conjugate to $\mathbf{d}^{(0)}, \mathbf{d}^{(1)}, \cdots, \mathbf{d}^{(k)}$. This is accomplished by choosing $\beta_k$ to be

$$\beta_k = \frac{\mathbf{g}^{(k+1)T}\mathbf{Q}\mathbf{d}^{(0)}}{\mathbf{d}^{(k)T}\mathbf{Q}\mathbf{d}^{(k)}}.$$

# Conjugate Direction Methods

- The conjugate gradient algorithm for quadratic problems



The conjugate gradient algorithm is summarized below.

1. Set $k := 0$; select the initial point $\mathbf{x}^{(0)}$.

2. $\mathbf{g}^{(0)} = \nabla f(\mathbf{x}^{(0)})$. If $\mathbf{g}^{(0)} = \mathbf{0}$, stop, else set $\mathbf{d}^{(0)} = -\mathbf{g}^{(0)}$.

3. $\alpha_k = -\frac{\mathbf{g}^{(k)T}\mathbf{d}^{(k)}}{\mathbf{d}^{(k)T}\mathbf{Q}\mathbf{d}^{(k)}}$.

4. $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}$.

5. $\mathbf{g}^{(k+1)} = \nabla f(\mathbf{x}^{(k+1)})$. If $g^{(k+1)} = \mathbf{0}$, stop.

6. $\beta_k = \frac{\mathbf{g}^{(k+1)T}\mathbf{Q}\mathbf{d}^{(0)}}{\mathbf{d}^{(k)T}\mathbf{Q}\mathbf{d}^{(k)}}$.

7. $\mathbf{d}^{(k+1)} = -\mathbf{g}^{(k+1)} + \beta_k \mathbf{d}^{(k)}$.

8. Set $k := k + 1$; go to step 3.

# Conjugate Direction Methods

- The conjugate gradient algorithm for quadratic problems

**Proposition 1.** *In the conjugate gradient algorithm, the directions* $\mathbf{d}^{(0)}, \mathbf{d}^{(1)}, \cdots, \mathbf{d}^{(n-1)}$ *are* $\mathbf{Q}$*-conjugate.*

Proof. By induction.

When there is no numerical error, the iteration of CG terminates when *k*=*n*−1.

**Lemma 1.**

$$\mathbf{g}^{(k+1)T}\mathbf{d}^{(i)} = 0$$

*for all* $k, 0 \leq k \leq n-1$, *and* $0 \leq i \leq k$.

Example: $\min_{\mathbf{x}} f(x_1, x_2, x_3) = \frac{3}{2}x_1^2 + 2x_2^2 + \frac{3}{2}x_3^2 + x_1x_3 + 2x_2x_3 - 3x_1 - x_3.$

# Conjugate Direction Methods

- The conjugate gradient algorithm for non-quadratic problems

For a general nonlinear function the Hessian is a matrix that has to be reevaluated at each iteration of the algorithm. This can be computationally very expensive. Thus, an efficient implementation of the conjugate gradient algorithm that eliminates the Hessian evaluation at each step is desirable.

Observe that $\mathbf{Q}$ appears only in the computation of the scalars $\alpha_k$ and $\beta_k$. Because

$$\alpha_k = \arg\min_{\alpha>0} f(\mathbf{x}^{(k)} + \alpha\mathbf{d}^{(k)}),$$

the closed form formula for $\alpha_k$ in the algorithm can be replaced by a numerical line search procedure. Therefore, we only need to concern ourselves with the formula for $\beta_k$.

# Conjugate Direction Methods

- The conjugate gradient algorithm for non-quadratic problems

Recall that in the quadratic case:

$$\beta_k = \frac{\mathbf{g}^{(k+1)T}\mathbf{Q}\mathbf{d}^{(k)}}{\mathbf{d}^{(k)T}\mathbf{Q}\mathbf{d}^{(k)}}.$$

Hessian-free

The *Hestenes-Stiefel* formula. It is based on replacing the term $\mathbf{Q}\mathbf{d}^{(k)}$ by the term $(\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)})/\alpha_k$.

The two terms are equal in the quadratic case, as we now show. $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}$. Premultiplying both sides by $\mathbf{Q}$, and recognizing that $\mathbf{g}^{(k)} = \mathbf{Q}\mathbf{x}^{(k)} - \mathbf{b}$, we get $\mathbf{g}^{(k+1)} = \mathbf{g}^{(k)} + \alpha_k \mathbf{Q}\mathbf{d}^{(k)}$, which we can rewrite as $\mathbf{Q}\mathbf{d}^{(k)} = (\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)})/\alpha_k$.

Substituting this into the original equation for $\beta_k$ gives

$$\beta_k = \frac{\mathbf{g}^{(k+1)T}[\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)}]}{\mathbf{d}^{(k)T}[\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)}]},$$

# Conjugate Direction Methods

- The conjugate gradient algorithm for non-quadratic problems

*The Polak-Ribiere formula.* Starting from the Hestenes-Stiefel formula, we multiply out the denominator to get

$$\beta_k = \frac{\mathbf{g}^{(k+1)T}[\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)}]}{\mathbf{d}^{(k)T}\mathbf{g}^{(k+1)} - \mathbf{d}^{(k)T}\mathbf{g}^{(k)}}. \tag{1}$$

By Lemma 1, $\mathbf{d}^{(k)T}\mathbf{g}^{(k+1)} = 0$. Also, since $\mathbf{d}^{(k)} = -\mathbf{g}^{(k)} + \beta_{k-1}\mathbf{d}^{(k-1)}$, and premultiplying this by $\mathbf{g}^{(k)T}$, we get

$$\mathbf{g}^{(k)T}\mathbf{d}^{(k)} = -\mathbf{g}^{(k)T}\mathbf{g}^{(k)} + \beta_{k-1}\mathbf{g}^{(k)T}\mathbf{d}^{(k-1)} = -\mathbf{g}^{(k)T}\mathbf{g}^{(k)},$$

where once again we used Lemma 1. Hence, we get

$$\beta_k = \frac{\mathbf{g}^{(k+1)T}[\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)}]}{\mathbf{g}^{(k)T}\mathbf{g}^{(k)}}.$$

# Conjugate Direction Methods

- The conjugate gradient algorithm for non-quadratic problems

*The Fletcher-Reeves formula.* Starting with the Polak-Ribiere formula, we multiply out the numerator to get

$$\beta_k = \frac{\mathbf{g}^{(k+1)T}\mathbf{g}^{(k+1)} - \mathbf{g}^{(k+1)T}\mathbf{g}^{(k)}}{\mathbf{g}^{(k)T}\mathbf{g}^{(k)}}.$$

We now use the fact that $\mathbf{g}^{(k+1)T}\mathbf{g}^{(k)} = 0$, which we get by using the equation

$$\mathbf{g}^{(k+1)T}\mathbf{d}^{(k)} = -\mathbf{g}^{(k+1)T}\mathbf{g}^{(k)} + \beta_{k-1}\mathbf{g}^{(k+1)T}\mathbf{d}^{(k-1)}$$

and applying Lemma 1. This leads to

$$\beta_k = \frac{\mathbf{g}^{(k+1)T}\mathbf{g}^{(k+1)}}{\mathbf{g}^{(k)T}\mathbf{g}^{(k)}},$$

# Conjugate Direction Methods

- Discussions

1. Reinitialize the direction vector to the negative gradient after every few iterations (e.g., $n$ or $n+1$)

2. If the line search is known to be inaccurate, the Hestenes-Stiefel formula for $\beta_k$ is recommended.

3. The choice of which formula for $\beta_k$ to use depends on the objective function.