Optimization Algorithms: Theory and Software Implementation

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Lecture: 30

This lecture concludes our discussion on the DFP method and introduces the BFGS method and the broader Broyden family of quasi-Newton algorithms. We begin by proving the final property of the DFP method concerning the preservation of positive definiteness.

Theorem: Consider minimizing a general function f using the DFP method where the step size α_k is chosen using an exact line search. If the matrix B_k is positive definite, then the updated matrix B_{k+1} is also positive definite.

Proof:

We aim to show that for any non-zero vector x, the quadratic form $x^TB_{k+1}x > 0$. Recall the DFP update formula:

$$B_{k+1} = B_k + (\delta_k\delta_k^T)/(\delta_k^T\gamma_k) - (B_k\gamma_k\gamma_k^TB_k)/(\gamma_k^TB_k\gamma_k)$$

The quadratic form is therefore:

$$x^TB_{k+1}x = x^TB_kx + (x^T\delta_k)^2/(\delta_k^T\gamma_k) - (x^TB_k\gamma_k)^2/(\gamma_k^TB_k\gamma_k)$$

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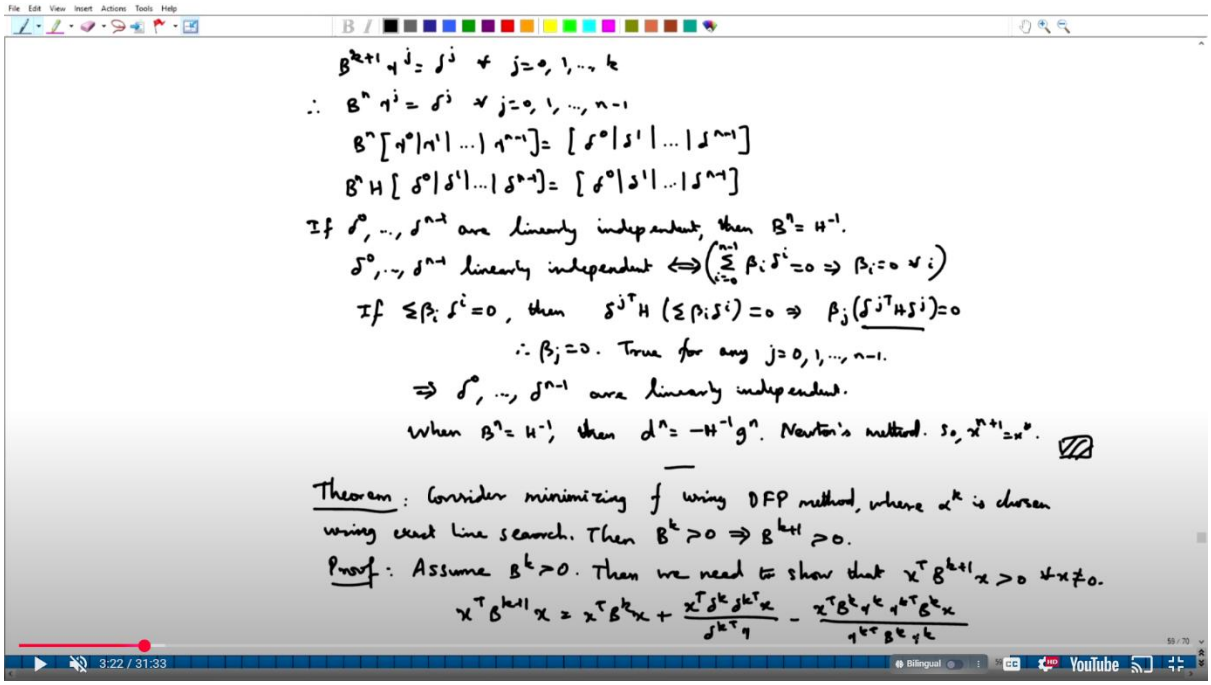

To analyze this expression, we define two vectors using the positive definite square root of B_k (which exists since B_k is positive definite):

$a = B_k^{1/2}x$

$b = B_k^{1/2}\gamma_k$

We can now rewrite the expression as:

$x^TB_{k+1}x = (a^Ta)(b^Tb)/(b^Tb) - (a^Tb)^2/(b^Tb) + (x^T\delta_k)^2/(\delta_k^T\gamma_k)$

$= [\ (a^Ta)(b^Tb) - (a^Tb)^2\ ] / (b^Tb) + (x^T\delta_k)^2/(\delta_k^T\gamma_k)$

By the **Cauchy-Schwarz inequality**, $(a^Tb)^2 \leq (a^Ta)(b^Tb)$, so the first term is non-negative. It equals zero if and only if a is parallel to b, i.e., $a = \lambda b$ for some scalar λ. This implies $B_k^{1/2}x = \lambda B_k^{1/2}\gamma_k$, and since $B_k^{1/2}$ is invertible, $x = \lambda\gamma_k$.

We now examine the denominator $\delta_k^T\gamma_k$. Given that an exact line search is used, we have the property that $\delta_k^Tg_{k+1} = 0$. Therefore:

$\delta_k^T\gamma_k = \delta_k^T(g_{k+1} - g_k) = -\delta_k^Tg_k$

Since $\delta_k = \alpha_kd_k$ and the search direction is $d_k = -B_kg_k$, this becomes:

$\delta_k^T\gamma_k = -\alpha_k(-B_kg_k)^Tg_k = \alpha_k\ g_k^TB_kg_k$

Because B_k is positive definite and $\alpha_k > 0$ for a minimization step, $g_k^TB_kg_k > 0$ for any non-zero g_k. Thus, $\delta_k^T\gamma_k > 0$.

Consequently, the second term, $(x^T\delta_k)^2/(\delta_k^T\gamma_k)$, is always non-negative and is zero only if

$x^T\delta_k = 0$.

Now, if $x^TB_{k+1}x = 0$, both terms in its expression must be zero. The first term is zero only if $x = \lambda\gamma_k$. Substituting this into the second term yields $(\lambda\gamma_k^T\delta_k)^2/(\delta_k^T\gamma_k) = \lambda^2(\delta_k^T\gamma_k)$, which is greater than zero for any non-zero λ (and hence any non-zero x). This is a contradiction. Therefore, $x^TB_{k+1}x$ cannot be zero for any non-zero x, and it must be strictly positive. This proves that B_{k+1} is positive definite.

This property highlights the importance of using an exact line search with the DFP method to ensure the descent property is maintained throughout the iterations.

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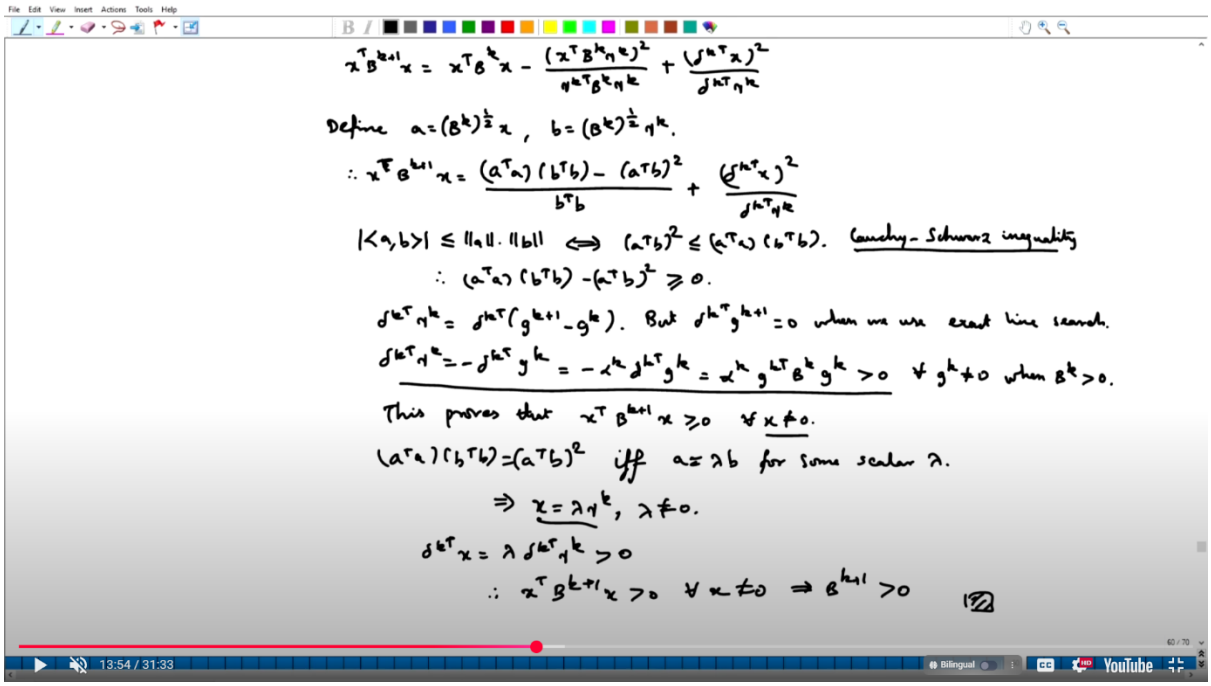

We now transition to the BFGS method, named after Broyden, Fletcher, Goldfarb, and Shanno. The BFGS update formula is given by:

$$B_{k+1} = B_k + [1 + (\gamma_k^T B_k \gamma_k)/(\delta_k^T \gamma_k)] * (\delta_k \delta_k^T)/(\delta_k^T \gamma_k) - (\delta_k \gamma_k^T B_k + B_k \gamma_k \delta_k^T)/(\delta_k^T \gamma_k)$$

The overall algorithm structure remains identical to the DFP and rank-one correction methods; only the update rule for B_k changes. The BFGS method also belongs to the **Broyden family** of updates, which can be expressed as a convex combination of the DFP and BFGS updates:

$$B_{k+1} = \varphi * B\{DFP\}_{k+1} + (1 - \varphi) * B\{BFGS\}_{k+1}$$

for some φ in the interval $[0, 1]$.

Setting $\varphi = 1$ gives the **DFP**

update, $\varphi = 0$ gives the **BFGS** update, and values in between yield a hybrid method.

Numerical experiments on quadratic functions show that all these methods—rank-one correction, DFP, BFGS, and the Broyden family—exhibit identical performance for these problems. They all converge to the exact solution in at most n steps and exactly compute the inverse Hessian H^{-1} upon completion.

For more general non-quadratic functions, such as

$$f(x_1, x_2) = x_1^2 e^{x_2} + x_2^2 e^{x_1},$$

the performance of these methods is also very similar. They successfully converge to a minimizer from some initial points (e.g., (1, 1) or (-0.5, -0.5)) but may converge to a saddle point from others (e.g., $(-\sqrt{2}, -\sqrt{2})$).

The rank-one correction method can sometimes be numerically unstable if the denominator $(\delta_k - B_k\gamma_k)^T\gamma_k$ becomes very small, which motivated the development of the more robust rank-two updates like DFP and BFGS.

This concludes our discussion on unconstrained optimization algorithms.

To summarize, we have covered:

1. **Gradient Descent:** $d_k = -\nabla f(x_k)$

2. **Conjugate Gradient (Fletcher-Reeves):** $d_0 = -g_0$, $d_k = -g_k + \beta_k d_{k-1}$

   where $\beta_k = (g_k^T g_k)/(g_{k-1}^T g_{k-1})$

3. **Newton's Method:** $d_k = -H_k^{-1} g_k$

4. **Damped Newton's Method:** Uses backtracking line search to choose α_k for the Newton direction.

5. **Modified Newton's Method:** $d_k = -(H_k + \lambda_k I)^{-1} g_k$, where λ_k is chosen to ensure the matrix is positive definite.

6. **Quasi-Newton Methods:** $d_k = -B_k g_k$, where B_k is updated to satisfy the quasi-Newton condition $B_{k+1}\gamma_k = \delta_k$ using various formulas (Rank-One, DFP, BFGS, Broyden Family).

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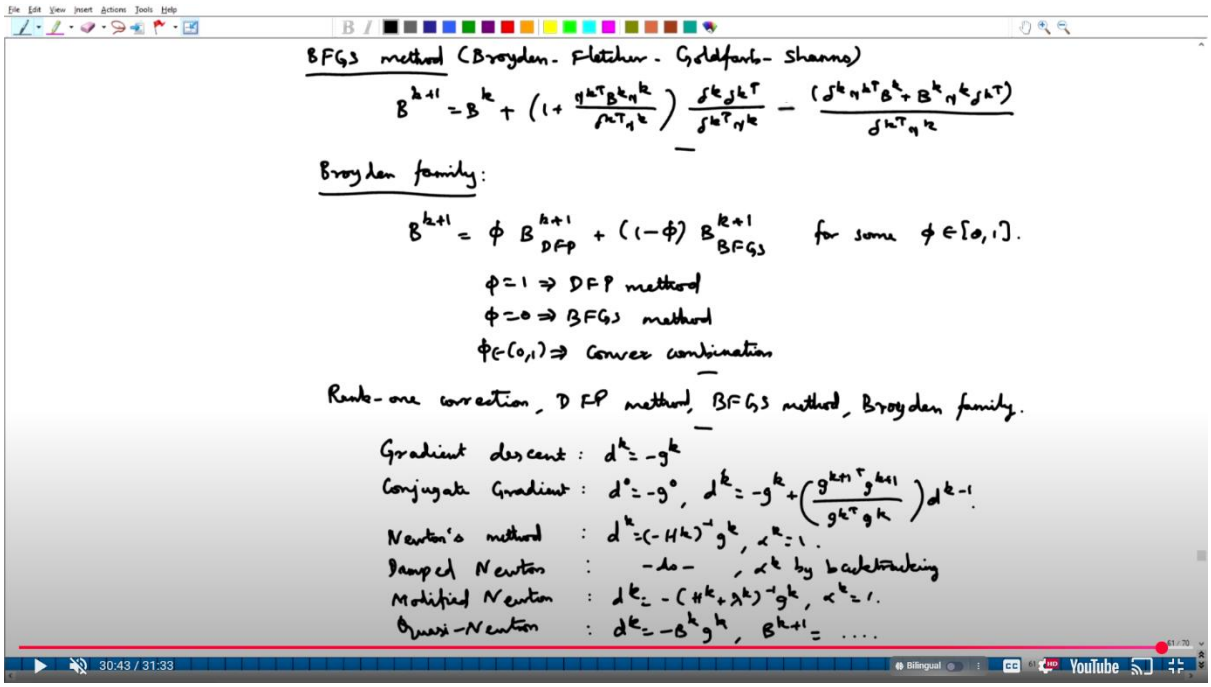

These foundational concepts are essential as we proceed to constrained optimization problems in the subsequent weeks. Thank you