Theoretical Background for Aerodynamic Shape Optimization

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Von Karman Institute
Brussels, Belgium
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LECTURE OUTLINE

• INTRODUCTION

• THEORETICAL BACKGROUND
  – SPIDER & FLY
  – BRACHISTOCHRONE

• SAMPLE APPLICATIONS
  – MARS AIRCRAFT
  – RENO RACER
  – GENERIC 747 WING/BODY

• DESIGN-SPACE INFLUENCE
THE SPIDER & THE FLY

- PROBLEM STATEMENT
- PROBLEM SET-UP
  - COST FUNCTION
  - DESIGN SPACE
  - GRADIENT & HESSIAN
- SEARCH METHODS
  - STEEPEST DESCENT
  - NEWTON ITERATION
  - NASH EQUILIBRIUM
- EXACT SOLUTION
THE SPIDER & THE FLY

Block Size
4" x 4" x 12"

Path Length
16.00"

Obvious Local-Minimum Path between Spider and Fly.
THE SPIDER & THE FLY

Block Size
4" x 4" x 12"

Path Length
$\sqrt{250.0}"$
$\sim 15.81"$

Non-Obvious Global-Minimum Path between Spider and Fly.
Path type to optimize is partitioned into four segments. Path described as the piecewise linear curve that connects:

\[(2, 0, 3), (X, 0, 4), (4, Y, 4), (4, 12, Z), (2, 12, 1)\].

Three design variables \((X, Y, Z)\), constrained by:

\[
\begin{align*}
0 & \leq X \leq 4, \\
0 & \leq Y \leq 12, \\
0 & \leq Z \leq 4.
\end{align*}
\]
SPIDER-FLY COST FUNCTION

Segment Lengths:

\[ S_1 = \left[ 1 + (X - 2)^2 \right]^\frac{1}{2}, \]
\[ S_2 = \left[ (X - 4)^2 + Y^2 \right]^\frac{1}{2}, \]
\[ S_3 = \left[ (Y - 12)^2 + (Z - 4)^2 \right]^\frac{1}{2}, \]
\[ S_4 = \left[ (Z - 1)^2 + 4 \right]^\frac{1}{2}. \]

Total Path Length:

\[ I \equiv S = S_1 + S_2 + S_3 + S_4. \]

Minimize \( I \) Subject to Constraints.
First Variation of Cost Function:

\[ \delta I = I_X \delta X + I_Y \delta Y + I_Z \delta Z \equiv G \delta \chi \]

\[ I_X = \frac{(X-2)}{S_1} + \frac{(X-4)}{S_2} \]

\[ I_Y = \frac{Y}{S_2} + \frac{(Y-12)}{S_3} \]

\[ G \equiv \text{Gradient Vector} \]

\[ \chi \equiv \text{Design Space Vector} \]

\[ I_Z = \frac{(Z-4)}{S_3} + \frac{(Z-1)}{S_4} \]
SPIDER-FLY HESSIAN MATRIX

\[
A = \begin{bmatrix}
I_{XX} & I_{YX} & I_{ZX} \\
I_{XY} & I_{YY} & I_{ZY} \\
I_{XZ} & I_{YZ} & I_{ZZ}
\end{bmatrix},
\]

\[
\begin{align*}
I_{XX} &= \frac{1}{S_1^3} + \frac{Y^2}{S_2^3} \\
I_{XY} &= I_{YX} = \frac{(4-X)Y}{S_2^3} \\
I_{XZ} &= I_{ZX} = 0 \\
I_{YY} &= \frac{(X-4)^2}{S_2^3} + \frac{(Z-4)^2}{S_3^3} \\
I_{YZ} &= I_{ZY} = \frac{(Y-12)(4-Z)}{S_3^3} \\
I_{ZZ} &= \frac{(Y-12)^2}{S_3^3} + \frac{4}{S_4^3}
\end{align*}
\]
Consider the Taylor series expansion of a function $f$.

\[ f(x + \Delta x) = f(x) + \Delta x f_x(x) + \frac{\Delta x^2}{2} f_{xx}(x) + \ldots + \frac{\Delta x^n}{n!} f_n(x) + \ldots \]

A first-order accurate approximation of $f_x(x)$ can be determined with the forward differencing formula

\[ f_x(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}. \]

Here $\Delta x$ is a small perturbation of the $X$ coordinate.
In the case of the spider-fly, let's approximate $I_X$.

$$I_X \simeq \frac{I(X + h, Y, Z) - I(X, Y, Z)}{h}$$

For example, using $h = 10^{-3}$ at $(X, Y, Z) = (2, 6, 2)$ gives:

$$I_X \simeq -0.31565661, \text{ an error of about 0.1\%.}$$

The exact value of $I_X$ at this location is $-\frac{2}{\sqrt{40}} \simeq -0.31622777$. 
Consider the Taylor series expansion of a complex function \( f \).

\[
f(x + \Delta x) = f(x) + \Delta x \ f_x(x) + \frac{\Delta x^2}{2} f_{xx}(x) + \ldots + \frac{\Delta x^n}{n!} f_n(x) + \ldots
\]

A second-order accurate approximation of \( f_x(x) \) can be found with the complex-variable formula

\[
f_x(x) \simeq \frac{Im[f(x + ih)]}{h}.
\]

Here \( \Delta x = ih \) is an imaginary perturbation of \( X \).
In the case of the spider-fly, let’s approximate $I_X$.

$$I_X \simeq \frac{Im[I(X + ih, Y, Z)]}{h}$$

For all $h \leq 10^{-3}$ at $(X, Y, Z) = (2, 6, 2)$, we get:

$$I_X \simeq -0.31622777.$$ 

This is identical to the exact value to 8 significant digits.
## GRADIENT APPROXIMATION

\[ \log_{10}(\text{Error } I_X) \]

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Stability of Finite-Difference and Complex-Variable Methods
Finite Difference vs Complex Variables

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{gradient_approximation}
\caption{Comparison of Finite Difference and Complex Variables methods for gradient approximation.}
\end{figure}
SPIDER-FLY SEARCH METHODS

Trajectory:

\[ \mathbf{x}^{n+1} = \mathbf{x}^n + \delta \mathbf{x}^n \]

Steepest Descent:

\[ \delta \mathbf{x}^n = -\lambda G, \quad \lambda > 0 \]
\[ \delta I^n = G \delta \mathbf{x}^n = -\lambda G^2 \leq 0 \]

Newton Iteration:

\[ \delta \mathbf{x}^n = -A^{-1}G = -HG \]
Rank-1 quasi-Newton:

\[ H^{n+1} = H^n + \frac{(\mathcal{P}^n)(\mathcal{P}^n)^T}{(\mathcal{P}^n)^T \delta G^n}, \]

where

\[ \delta G^n = G^{n+1} - G^n \]

and

\[ \mathcal{P}^n = \delta \chi^n - H^n \delta G^n. \]
Nash Equilibrium:

\[
\begin{align*}
\text{minimize } I(X^*, Y^n, Z^n) & \implies I_x(X^*, Y^n, Z^n) = 0 \implies X^*, \\
\text{minimize } I(X^n, Y^*, Z^n) & \implies I_x(X^n, Y^*, Z^n) = 0 \implies Y^*, \\
\text{minimize } I(X^n, Y^n, Z^*) & \implies I_x(X^n, Y^n, Z^*) = 0 \implies Z^*.
\end{align*}
\]

These reduce to:

\[
\begin{align*}
X^* &= \frac{2(2 + Y^n)}{1 + Y^n}, & Y^* &= \frac{12(4 - X^n)}{8 - X^n - Z^n}, & Z^* &= 4 - \frac{3(12 - Y^n)}{14 - Y^n}.
\end{align*}
\]

Update design vector:

\[
[X_n^{n+1}, Y_n^{n+1}, Z_n^{n+1}]^T = [X^*, Y^*, Z^*]^T
\]
**SPIDER-FLY INITIAL PATH**

\[
\chi^0 = \begin{bmatrix} 2 \\ 6 \\ 2 \end{bmatrix}, \quad G^0 = \begin{bmatrix} \frac{-2}{\sqrt{40}} \\ 0.0 \\ \left(\frac{-3}{\sqrt{40}} + \frac{1}{\sqrt{5}}\right) \end{bmatrix} \approx \begin{bmatrix} -0.31623 \\ 0.0 \\ -0.02713 \end{bmatrix},
\]

\[
A^0 \approx \begin{bmatrix} 1.14230 & 0.04743 & 0.0 \\ 0.04743 & 0.03162 & -0.04743 \\ 0.0 & -0.04743 & 0.50007 \end{bmatrix},
\]

\[
I^0 = (1 + 2\sqrt{40} + \sqrt{5}) \approx 15.88518
\]
Initial Path between Spider and Fly.
Convergence of Gradient for Steepest Descent.
Steepest-Descent Trajectory through Design Space.
Convergence of Gradient for Newton Iteration.

Vassberg & Jameson, VKI Lecture-I, Brussels, 7 April, 2014
Newton-Iteration Trajectory through Design Space.
### Convergence of Newton Iteration on the Spider-Fly Problem.

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Convergence of Gradient for Rank-1 quasi-Newton Iteration.
Rank-1 quasi-Newton Trajectory through the Design Space.
### SPIDER-FLY RANK-1 QUASI-NEWTON

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Convergence of Rank-1 quasi-Newton on Spider-Fly.
### SPIDER-FLY RANK-1 QUASI-NEWTON

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Convergence of Rank-1 quasi-Newton on Spider-Fly.
### SPIDER-FLY RANK-1 QUASI-NEWTON

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Convergence of Rank-1 quasi-Newton on Spider-Fly.
Convergence of Rank-1 quasi-Newton on Spider-Fly.

Vassberg & Jameson, VKI Lecture-I, Brussels, 7 April, 2014
### SPIDER-FLY RANK-1 QUASI-NEWTON

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Convergence of Rank-1 quasi-Newton on Spider-Fly.
SPIDER-FLY NASH EQUILIBRIUM

Convergence of Error for Nash Equilibrium.
Convergence of Gradient for Nash Equilibrium.
Nash Equilibrium Trajectory through the Design Space.
**Convergence of Nash Equilibrium on Spider-Fly.**

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SPIDER-FLY GEODESIC

Super Ellipsoid Surface:

\[
\left(\frac{|x-2|}{2}\right)^p + \left(\frac{|y-6|}{6}\right)^p + \left(\frac{|z-2|}{2}\right)^p = 1, \quad p \geq 2
\]

Spider Initial Position: \hspace{1cm} Trapped Fly Position:

\[
\begin{align*}
XS &= 2 \\
YS &= 6 \left[ 1 - \left[ 1 - \frac{1}{2^p} \right]^{\frac{1}{p}} \right] \\
ZS &= 3
\end{align*}
\hspace{1cm}
\begin{align*}
XF &= 2 \\
YF &= 12 - YS \\
ZF &= 1
\end{align*}
\]
SPIDER-FLY OBSERVATIONS

- **CHOICE OF PATH**
  - WOODEN BLOCK vs SUPER ELLIPSOID
  - DEFINES COST FUNCTION & DESIGN SPACE
  - DISCRETE vs CONTINUUM

- **CHOICE OF SEARCH METHOD**
  - N.I. 3(1 + 3) << 295 S.D. → GOOD TRADE
  - HESSIAN COST = $O(N) \times \text{GRADIENT COST}$
  - LARGE $N$ → AVOID NEWTON ITERATION
Obvious Local-Minimum Path between Spider and Fly.
Obvious Local-Minimum Path on Flattened Box.
SPIDER-FLY EXACT SOLUTION

Non-Obvious Global-Minimum on Flattened Box.

Block Size
4" x 4" x 12"

Path Length
$\sqrt{250.0}$"
~ 15.81"
Non-Obvious Global-Minimum Path between Spider and Fly.
BRACHISTOCHRONE PROBLEM

• GRADIENT & HESSIAN
• BRACHISTOCHRONE
• GRADIENT CALCULATIONS
• SEARCH METHODS
• RESULTS
• SUMMARY
Consider the class of optimization problems with cost function

\[ I = \int_{x_0}^{x_1} F(x, y, y') \, dx \]  

(1)

where \( F \) is an arbitrary, twice-differentiable function, and \( y(x) \) is the trajectory between fixed end points to be optimized.

The first variation of the cost function is

\[ \delta I = \int_{x_0}^{x_1} G \, \delta y \, dx. \]  

(2)

Under a variation \( \delta y \), the resulting variation in \( I \) is

\[ \delta I = \int_{x_0}^{x_1} \left( \frac{\partial F}{\partial y} \delta y + \frac{\partial F}{\partial y'} \delta y' \right) \, dx. \]
Integrating the second term by parts with fixed end points gives

$$\delta I = \int_{x_0}^{x_1} G(x) \delta y(x) \, dx$$

where

$$G = \frac{\partial F}{\partial y} - \frac{d}{dx} \frac{\partial F}{\partial y'}.$$ (3)

Also,

$$\delta G = A \delta y$$

where $A$ is the Hessian.
The first variation of the gradient can be written as
\[
\delta G = \frac{\partial G}{\partial y} \delta y + \frac{\partial G}{\partial y'} \delta y' + \frac{\partial G}{\partial y''} \delta y''.
\]

The Hessian can be represented as the local differential operator
\[
A = \frac{\partial G}{\partial y} + \frac{\partial G}{\partial y'} \frac{d}{dx} + \frac{\partial G}{\partial y''} \frac{d^2}{dx^2}.
\]

One might also represent the Hessian by the integral operator
\[
\delta G(x) = \int_{x_0}^{x_1} a(x, \xi) \delta y(x) \, d\xi.
\]
The brachistochrone problem is the determination of path \( y(x) \) connecting points \((x_0, y_0)\) and \((x_1, y_1)\) such that the time taken by a particle traversing this path, subject only to the force of gravity, is a minimum. The total time is given by

\[
T = \int_{x_0}^{x_1} \frac{ds}{v}
\]

where the velocity of a particle falling under the influence of gravity, \( g \), and starting from rest at \( y = 0 \), is \( v = \sqrt{2gy} \).
Setting \( ds = \sqrt{(1 + y'^2)} \, dx \), one finds that

\[
T = \frac{I}{\sqrt{2g}}
\]

where

\[
I = \int_{x_0}^{x_1} F(y, y') \, dx
\]

with

\[
F(y, y') = \sqrt{\frac{1 + y'^2}{y}}.
\]
Under a variation $\delta y$, the resulting variation in $I$ is

$$\delta I = \int_{x_0}^{x_1} \left( \frac{\partial F}{\partial y} \delta y + \frac{\partial F}{\partial y'} \delta y' \right) dx.$$ 

Integrating the second term by parts with fixed end points

$$\delta I = \int_{x_0}^{x_1} G(x) \delta y(x) dx$$

where

$$G = \frac{\partial F}{\partial y} - \frac{d}{dx} \frac{\partial F}{\partial y'} = -\sqrt{1 + y'^2} - \frac{d}{dx} \frac{y'}{\sqrt{y(1 + y'^2)}}.$$
This may be simplified to

\[ G = -\frac{1 + y'^2 + 2yy''}{2(y(1 + y'^2))^{\frac{3}{2}}}. \]  

(7)

In this case, since \( F \) is not a function of \( x \),

\[ \left( y' \frac{\partial F}{\partial y'} - F \right)' = y'' \frac{\partial F}{\partial y'} + y' \frac{d}{dx} \frac{\partial F}{\partial y'} - \frac{\partial F}{\partial y} y'' - \frac{\partial F}{\partial y} y' \]

\[ = y' \left( \frac{d}{dx} \frac{\partial F}{\partial y'} - \frac{\partial F}{\partial y} \right) = -y' G. \]
On the optimal path \( G = 0 \) and hence

\[
\left( y' \frac{\partial F}{\partial y'} - F \right) \text{ is constant.}
\]

It follows that \( \sqrt{y(1 + y'^2)} = C \), where \( C \) is a constant.

The classical solution to the brachistochrone is a cycloid.

\[
x(t) = \frac{1}{2}C^2(t - \sin(t))
\]

\[
y(t) = \frac{1}{2}C^2(1 - \cos(t))
\]
GRADIENT CALCULATIONS

- CONTINUOUS GRADIENT
  - Approximation of the Exact Gradient

- DISCRETE GRADIENT
  - Exact Derivative of Discrete Function
CONTINUOUS GRADIENT

The exact continuous gradient of Eqn (7) is approximated by

\[ G_j = - \frac{1 + y_j'^2 + 2y_jy_j''}{2(y_j(1 + y_j'^2))^{\frac{3}{2}}} \]  

(8)

where

\[ y_j' = \frac{y_j + 1 - y_j - 1}{2\Delta x} \quad , \quad y_j'' = \frac{y_j + 1 - 2y_j + y_j - 1}{\Delta x^2}. \]
The exact cost function of Eqn (6) can be approximated by

$$I_R = \sum_{j=0}^{N} F_{j+\frac{1}{2}} \Delta x$$

where

$$F_{j+\frac{1}{2}} = \sqrt{1 + y_j'^2 \frac{1 + y_{j+\frac{1}{2}}}{y_{j+\frac{1}{2}}}}$$

$$y_{j+\frac{1}{2}} = \frac{1}{2}(y_{j+1} + y_j)$$

$$y_j' = \frac{y_{j+1} - y_j}{\Delta x},$$
Differentiating Eqn (9) gives another approximate form for the gradient as

\[ G_j = \frac{\partial I_R}{\partial y_j} = B_j - \frac{1}{2} - B_{j+\frac{1}{2}} - \frac{\Delta x}{2}(A_{j+\frac{1}{2}} + A_{j-\frac{1}{2}}) \]  

(10)

where

\[ A_{j+\frac{1}{2}} = \frac{1 + y_{j+\frac{1}{2}}^2}{2y_{j+\frac{1}{2}}^2} \]
\[ B_{j+\frac{1}{2}} = \frac{y_{j+\frac{1}{2}}}{\sqrt{y_{j+\frac{1}{2}}^2 + (1 + y_{j+\frac{1}{2}}^2)}}. \]
SEARCH METHODS

- STEEPEST DESCENT
- SMOOTHED STEEPEST DESCENT
- IMPLICIT DESCENT
- MULTIGRID DESCENT
- KRYLOV ACCELERATION
- QUASI-NEWTON METHODS
  - Rank 1
  - Davidon-Fletcher-Powell (DFP)
  - Broyden-Fanno-Goldfarb-Shannon (BFGS)
STEEPEST DESCENT

Forward Euler step gives
\[ y_j^{n+1} = y_j^n - \lambda G^n_j, \quad \lambda > 0 \]
\[ \delta y^n = -\lambda G^n. \]

Then to first order the variation in \( I \) is
\[ \delta I = \int_{x_0}^{x_1} G \delta y dx = -\lambda \int_{x_0}^{x_1} G^2 dx \]
and
\[ \delta I \leq 0. \]
STEEPEST DESCENT

This may be regarded as a forward Euler discretization of a time dependent process with $\lambda = \Delta t$. Hence, $\frac{\partial y}{\partial t} = -G$. Substituting for $G$ from Eqn (7), $y$ solves the nonlinear parabolic equation

$$\frac{\partial y}{\partial t} = \frac{1 + y'^2 + 2yy''}{2y(1 + y'^2)^{3/2}}. \quad (11)$$

The time step limit for stable integration is dominated by the parabolic term $\beta y''$, where $\beta = \frac{y}{(y(1+y'^2))^{3/2}}$.

This gives the following estimate on the time step limit.

$$\Delta t^* = \frac{\Delta x^2}{2\beta}.$$
Define $\bar{g}$ with the implicit smoothing equation.

$$\bar{g} - \frac{\partial}{\partial x} \epsilon \frac{\partial \bar{g}}{\partial x} = g$$

(12)

Now set

$$\delta y = -\lambda \bar{g}.$$  

(13)

Then to first order the variation in $I$ is

$$\delta I = \int_{x_0}^{x_1} g \delta y dx = -\lambda \int_{x_0}^{x_1} \left( \bar{g} - \frac{\partial}{\partial x} \epsilon \frac{\partial \bar{g}}{\partial x} \right) \bar{g} dx.$$
Integrating by parts and noting that the end points are fixed,

\[ \delta I = -\lambda \int_{x_0}^{x_1} \left( \bar{g}^2 + \epsilon \left( \frac{\partial \bar{g}}{\partial x} \right)^2 \right) dx. \]

Again,

\[ \delta I \leq 0. \]
IMPLICIT DESCENT

If the gradient is dominated by a $y''$ term, the smoothed descent given by Eqn (13) can be made equivalent to an implicit scheme.

Consider the parabolic equation, $\frac{\partial y}{\partial t} = \beta \frac{\partial^2 y}{\partial x^2}$, where $\beta$ is variable.

The system for an implicit scheme is

$$-\alpha \delta y_{j-1} + (1 + 2\alpha) \delta y_j - \alpha \delta y_{j+1} = -\Delta t \hat{G}_j$$

(14)

where $\delta y_j$ is the correction to $y_j$,

$$\alpha = \frac{\beta \Delta t}{\Delta x^2} = \frac{\Delta t}{2 \Delta t^*}$$

(15)
Combining Eqns (12 & 13), the discrete smoothed descent method assumes the form of Eqn (14) with

\[ \alpha = \frac{\epsilon}{\Delta x^2}. \]  

Comparing Eqn (15) with Eqn (16), one can see using the smoothed gradient is equivalent to an implicit time stepping scheme if \( \epsilon = \beta \Delta t \). Furthermore, a Newton iteration is recovered as \( \Delta t \to \infty \).
MULTIGRID DESCENT

Consider a sequence of $K$ meshes, generated by eliminating alternate points along each coordinate direction of mesh-level $k$ to produce mesh-level $k + 1$. Note that $k = 1$ refers to the finest mesh of the sequence. In order to give a precise description of the multigrid scheme, subscripts may be used to indicate grid level. Several transfer operations need to be defined. First, the solution vector, $y$, on grid $k$ must be initialized as

$$y_k^{(0)} = T_{k,k-1} y_{k-1}, \quad 2 \leq k \leq K$$

where $y_{k-1}$ is the current value of the solution on grid $k-1$, and $T_{k,k-1}$ is a transfer operator.
It is also necessary to transfer a residual forcing function, \( P \), such that the solution on grid \( k \) is driven by the residuals of grid \( k-1 \). This can be accomplished by setting

\[
P_k = Q_{k,k-1} \mathcal{G}_{k-1}(y_{k-1}) - \mathcal{G}_k(y_k^{(0)}),
\]

where \( Q_{k,k-1} \) is another transfer operator. Now, \( \mathcal{G}_k \) is replaced by \( \mathcal{G}_k + P_k \) in the time-stepping such that

\[
y_k^+ = y_k^{(0)} - \Delta t_k \left[ \mathcal{G}_k(y_k) + P_k \right]
\]

where the superscript \( + \) denotes the updated value. The resulting solution vector, \( y_k^+ \), provides the initial data for grid \( k + 1 \).
Finally, the accumulated correction on grid $k$ is transferred back to grid $k - 1$ with the aid of an interpolation operator, $I_{k-1,k}$. Thus one sets

$$y_{k-1}^{++} = y_{k-1}^+ + I_{k-1,k} \left( y_{k}^{++} - y_{k}^{(0)} \right)$$

where the superscript $^{++}$ denotes the result of both the time step on grid $k$ and the interpolated correction from grid $k + 1$. 
MULTIGRID DESCENT

Three-Level Multigrid W-Cycle

$k = 1$

$k = 2$

$k = 3$

Three-Level Multigrid W-Cycle
MULTIGRID DESCENT

Recursive Stencil for a $K$-Level Multigrid W-Cycle

$(K - 1)$-Level W-Cycle

$(K - 1)$-Level W-Cycle

Recursive Stencil for a $K$-Level Multigrid W-Cycle
In a three-dimensional setting, the number of cells is reduced by a factor of 8 on each coarser grid. By examination of the stencils, it can be verified that the work of one multigrid $W$-Cycle, in work units, is on the order of

$$1 + \frac{2}{8} + \frac{4}{64} + \ldots + \frac{1}{4^K} < \frac{4}{3}.$$  

Hence, one multigrid $W$-Cycle only requires about $\frac{1}{3}$ more effort as that required for a fine-mesh iteration.
KRYLOV ACCELERATION

Given \( K \) linearly independent \((y, G)\) vectors, one can survey the \( K\)-dimensional subspace spanned by these vectors.

\[
y^* = \sum_{k=1}^{K} \gamma_k y^k, \quad G^* = \sum_{k=1}^{K} \gamma_k G^k, \quad \sum_{k=1}^{K} \gamma_k = 1
\]

Minimize the \( L_2 \) Norm of \( G^* \) to determine the recombination coefficients \( \gamma_k \).

Now,

\[
y_{j}^{n+1} = y_j^* - \lambda G_j^*
\]
Quasi-Newton methods estimate the Hessian, $A$, or its inverse $A^{-1}$, from changes $\delta G$ in the gradient during the search steps. By the definition of $A$, to first order

$$\delta G = A \delta y$$

Let $H^n$ be an estimate of $A^{-1}$ at the $n^{th}$ step. Then it should be required to satisfy

$$H^n \delta G^n = \delta y^n$$

This can be satisfied by various recursive formulas for $H$. 
QUASI-NEWTON METHODS

Rank 1

\[ H^{n+1} = H^n + \frac{p^n(p^n)^T}{(p^n)^T \delta G^n} \]

where

\[ p^n = \delta y^n - H^n \delta G^n \]
QUASI-NEWTON METHODS

Davidon-Fletcher-Powell (DFP)

\[ H^{n+1} = H^n + \frac{\delta y^n (\delta y^n)^T}{(\delta y^n)^T \delta G^n} - \frac{H^n \delta G^n (\delta G^n)^T H^n}{(\delta G^n)^T H^n \delta G^n} \]
QUASI-NEWTON METHODS

Broyden-Fanno-Goldfarb-Shannon (BFGS)

\[ H^{n+1} = H^{n} + \left( 1 + \frac{(\delta G^n)^T H^{n} \delta G^n}{(\delta G^n)^T \delta y^n} \right) \frac{\delta y^n (\delta y^n)^T}{(\delta G^n)^T \delta y^n} \]

\[ - \frac{H^n \delta G^n (\delta y^n)^T}{(\delta G^n)^T \delta y^n} + \delta y^n (\delta G^n)^T H^n \]
RESULTS

• ACCURACY OF GRADIENTS
  – Continuous vs. Discrete
  – Level of Accuracy
  – Order of Accuracy

• PERFORMANCE OF SEARCH METHODS
  – Build-up of Explicit Schemes
  – Comparison with Implicit Scheme
  – Grid-Independent Convergence
  – Tested with up to 8192 Design Variables

• ROBUSTNESS
Convergence of continuous gradient, implicit scheme, N=31.
Convergence of discrete gradient, implicit scheme, N=31.
Convergence of continuous gradient, implicit scheme, N=511.
Computed path errors as a function of mesh size.
Difference of measurable cost function between gradients.
PERFORMANCE: STEEPEST DESCENT

History of paths of steepest descent, N=31.
Convergence history of steepest descent, $N=31$. 

Vassberg & Jameson, VKI Lecture-I, Brussels, 7 April, 2014
PERFORMANCE: SMOOTHED DESCENT

History of paths of smoothed descent, N=31 & STEP=100.
Convergence history of smoothed descent, N=31.
This document discusses the performance of Krylov acceleration in the context of a graph. The graph shows a history of paths for Krylov acceleration with $N=31$ and $STEP=100$. The graph includes lines labeled 'Exact', 'cyc 1', 'cyc 2', 'cyc 4', 'cyc 8', 'cyc 32', and 'cyc 64'. The x-axis represents a range from 0.1 to 1.0, while the y-axis ranges from -0.65 to -0.30.
PERFORMANCE: KRYLOV ACCELERATION

Convergence history of Krylov acceleration, N=31.
PERFORMANCE: MULTIGRID DESCENT

History of paths for multigrid acceleration, N=31.
PERFORMANCE: MULTIGRID DESCENT

Convergence history of multigrid acceleration, N=31.
PERFORMANCE: IMPLICIT DESCENT

History of paths of implicit stepping, N=31.
Convergence history of implicit stepping, N=31.
PERFORMANCE: IMPLICIT DESCENT

History of paths of implicit stepping, \( N=511 \).
PERFORMANCE: IMPLICIT DESCENT

Convergence history of implicit stepping, N=511.
PERFORMANCE: MULTIGRID vs. IMPLICIT

Comparison of grid-independent convergence histories.

Vassberg & Jameson, VKI Lecture-I, Brussels, 7 April, 2014
History of paths for Rank-1 quasi-Newton, N=31.
Comparison of quasi-Newton convergence histories, N=31.
PERFORMANCE: QUASI-NEWTON

History of paths for Rank-1 quasi-Newton, N=511.
Comparison of quasi-Newton convergence histories, N=511.
Comparison of convergence dependencies on dimensionality.
SUMMARY: BRACHISTOCHRONE STUDY

- **COMPARISON OF GRADIENTS**
  - Both Gradients Exhibited $2^{nd}$-Order Accuracy
  - Continuous Gradient Slightly More Accurate

- **SEARCH METHODS**
  - Steepest Descent Scales with $N^2$
  - Quasi-Newton Methods Scale with $N$
  - Implicit Scheme Independent of $N$
  - Multigrid Descent Independent of $N$
  - Smoothed Descent Equivalent to Implicit Scheme
Theoretical Background for Aerodynamic Shape Optimization

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