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Comparison between the fitness function and its best quadratic approximation

The standard method to estimate the fitness landscape is the approach of Lande and Arnold (1983), which has been very widely used and has over 1000 citations. Basically, what they do is to estimate the actual fitness function as its best quadratic approximation (BQA) given data which is a set of phenotypic character variables and observed fitness such as the number of off springs. We show that the "best" quadratic approximation is futile and does not provide the true information a fitness function can convey, because it often approximates the true fitness function only poorly. More often than not, we would find that the BQA displays artifacts rather than the actual characteristic of fitness landscape of biological interest.

I have tested Lande-Arnold method in there scenarios: fitness function is unimodal in one and two dimensions and univariate bimodal fitness function. In each case, I picked some graphs that can indicate how poorly best quadratic approximation estimates different fitness functions of biological interest. Those graphs on the following pages were made in R and can be reproduced using the code I wrote.

Given the Lande-Arnold method which assumes $\mathbf{Z}$ is multivariate normal with mean vector $\boldsymbol{\mu} = \mathbf{0}$, variance matrix A_1 and its Probability density function(PDF):

$$f(\boldsymbol{z}) = c_1 \exp\left\{-\frac{1}{2}(\boldsymbol{z}-\boldsymbol{\mu})^T {A_1}^{-1}(\boldsymbol{z}-\boldsymbol{\mu})\right\}$$

and g(z) is true fitness function from which we can get the best quadratic function as follows:

$$g_2(\boldsymbol{z}) = \alpha + \boldsymbol{z}^T\beta + \frac{1}{2}z^T\gamma\boldsymbol{z}$$

where $\beta = E\left(\nabla g(\boldsymbol{z})\right)$, $\gamma = \mathrm{E}(\nabla^2 \mathrm{g}(\boldsymbol{z}))$ (Charles J. Geyer, Ruth G. Shaw. 2008)

By definition $1 = E\left(g_2(\boldsymbol{z})\right) = E(\alpha) + E(\boldsymbol{z}^T\beta) + E(\frac{1}{2}\boldsymbol{z}^T\gamma\boldsymbol{z})$ because z is multivariate with mean vector 0, $E(\boldsymbol{z}^T\beta) = 0$. $E\left(\frac{1}{2}\boldsymbol{z}^T\gamma\boldsymbol{z}\right) = \frac{1}{2}E(\boldsymbol{z}^T\gamma\boldsymbol{z}) = \frac{1}{2}trace\left(E(\gamma\boldsymbol{z}\boldsymbol{z}^T)\right) = \frac{1}{2}sum(\gamma \times A_1)$ (" $\times$ " means multiplication component wise)

Unimodal

We assume the fitness function $g(z)$ is unimodal and has the form

$$g(\boldsymbol{z}) = c_2 \exp\left\{-\frac{1}{2}(\boldsymbol{z}-\boldsymbol{\mu_2})^T {A_2}^{-1}(\boldsymbol{z}-\boldsymbol{\mu_2})\right\}$$

$$g(\boldsymbol{z})f(\boldsymbol{z}) = c_3 \exp\left\{-\frac{1}{2}(\boldsymbol{z}-\boldsymbol{\mu_3})^T {A_3}^{-1}(\boldsymbol{z}-\boldsymbol{\mu_3})\right\}$$

where ${A_3}^{-1} = {A_1}^{-1} + {A_2}^{-1}$, $\boldsymbol{\mu_3} = A_3({A_1}^{-1}\boldsymbol{\mu_1} + {A_2}^{-1}\boldsymbol{\mu_2}$

In order to make $g(\boldsymbol{z})$a fitness function, $g(\boldsymbol{z})f(\boldsymbol{z})$has to integrate to 1, c_3 is the normalizing constant of the multivariate normal density with mean vector $\boldsymbol{\mu_3}$ and variance matrix A_3

Univariate

If z is univariate normal and we replace $A_i\ by\ v_i$, we can get

$$\beta = \frac{\mu_2}{v_1 + v_2} \quad , \quad \gamma = -\frac{1}{v_1 + v_2} + \beta^2 \, , \qquad \alpha = 1 - \frac{\gamma v_1}{2}$$

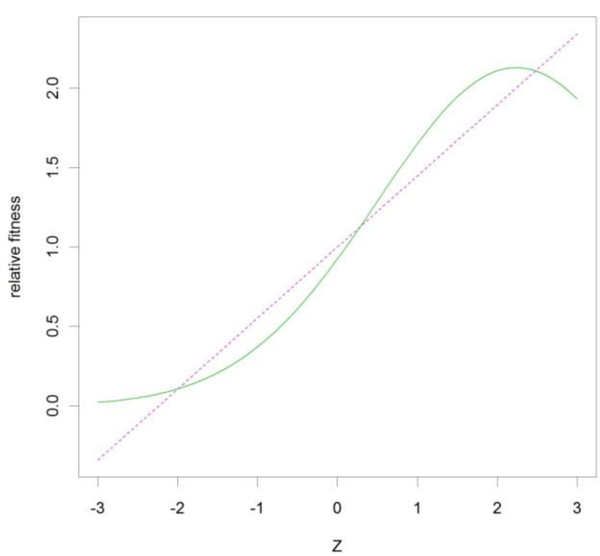
The BQA is

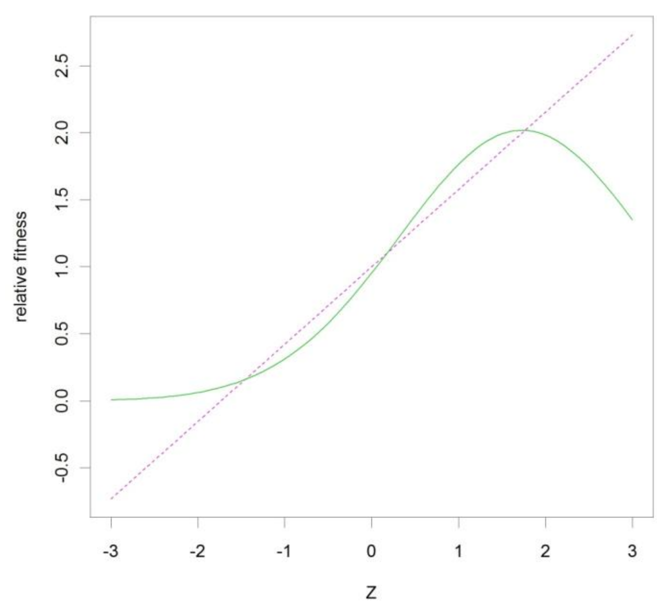
$$g_2(z) = \alpha + z\beta + \frac{1}{2} z^2 \gamma$$

It is not hard to notice that if we simply set $\gamma = 0$, then the BQA would become a linear function.

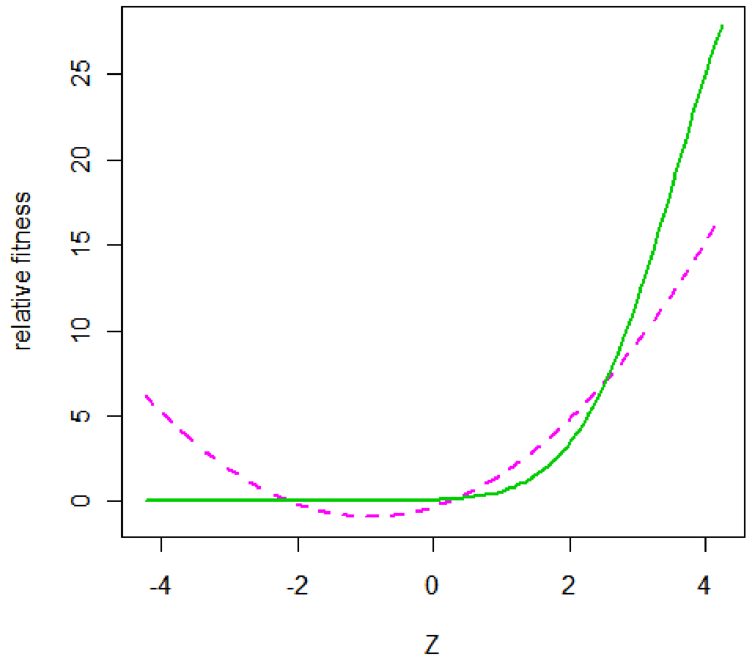
$$\gamma = -\frac{1}{v_1 + v_2} + \beta^2 = -\frac{\mu_2^2 - v_1 - v_2}{(v_1 + v_2)^2} = 0 \qquad \rightarrow \qquad \mu_2^2 = v_1 + v_2$$

BQA becomes linear when $\mu_2^2 = v_1 + v_2$, and the approximation to the fitness function would fall apart and yield very bad artifacts. It's like trying to use a straight line to study a parabola. It's simply not a good fit.





Even if μ_2 does not approximately equal to the square root of v1+v2, the BQA can still do a bad job, like the **Figure 3** to the right



Bimodal

We assume the fitness function g(z) is bimodal and has the form

$$g(z) = c\left\{\mathrm{p}_1 \frac{1}{\sqrt{2\pi \mathrm{v}_2}} \exp\left\{-\frac{1}{2}\frac{(z-\mu_2)^2}{v_2}\right\} + \mathrm{p}_2 \frac{1}{\sqrt{2\pi \mathrm{v}_3}} \exp\left\{-\frac{1}{2}\frac{(z-\mu_3)^2}{v_3}\right\}\right\}$$

where $\mathrm{p}_1 + \mathrm{p}_2 = 1, \quad 0 < \mathrm{p}_2 < 1$

Z is univariate normal, thus f(z) is still the same: $f(z) = \frac{1}{\sqrt{2\pi v_1}}\exp(-\frac{z^2}{2v_1})$

In order to calculate β *and* γ , we need to get $g^{'}(z)$ *and* $g^{''}(z)$

For the convenience of simplification, we make $c_1 = \frac{1}{\sqrt{2\pi v_1}}$, $c_2 = \mathrm{p}_1 \frac{1}{\sqrt{2\pi \mathrm{v}_2}}$, $c_3 = \mathrm{p}_2 \frac{1}{\sqrt{2\pi \mathrm{v}_3}}$

$$g^{'}(z) = -c\left\{c_2 \exp\left\{-\frac{1}{2}\frac{(z-\mu_2)^2}{v_2}\right\}\frac{(z-\mu_2)}{v_2} + c_3 \exp\left\{-\frac{1}{2}\frac{(z-\mu_3)^2}{v_3}\right\}\frac{(z-\mu_3)}{v_3}\right\}$$

$\beta = E\left(g'(z)\right) = \int f(z)g'(z)\,dz = c * \{(1) + (2)\}$

$(1) =$

$-\frac{c_1 c_2}{v_2}\int zexp(-\frac{(v_1+v_2)z^2-2\mu_2 v_1 z+\mu_2{}^2 v_1}{2v_1 v_2})\,dz + \frac{\mu_2 c_1 c_2}{v_2}\int exp(-\frac{(v_1+v_2)z^2-2\mu_2 v_1 z+\mu_2{}^2 v_1}{2v_1 v_2})\,dz$

$(2) =$

$-\frac{c_1 c_3}{v_3}\int zexp(-\frac{(v_1+v_3)z^2-2\mu_3 v_1 z+\mu_3{}^2 v_1}{2v_1 v_3})\,dz + \frac{\mu_3 c_1 c_3}{v_3}\int exp(-\frac{(v_1+v_3)z^2-2\mu_3 v_1 z+\mu_3{}^2 v_1}{2v_1 v_3})\,dz$

If $x \to \exp(ax^2 + bx + c)$ $\;and\; a < 0$, then $\mu = -\frac{b}{2a}$ $, \sigma^2 = -\frac{1}{2a}$ (Charles J. Geyer)

We apply this lemma to (1), (2) and get $\mu = \frac{\mu_2 v_1}{v_1+v_2}$ $, \sigma^2 = \frac{v_1 v_2}{v_1+v_2}$

$$(1) = \left\{\frac{\mu_2 \mathrm{p}_1}{(v_1+v_2)}\sqrt{\frac{1}{(v_1+v_2)2\pi}}\exp(-\frac{\mu_2{}^2}{2(v_1+v_2)})\right\}$$

$$(2) = \left\{\frac{\mu_3 \mathrm{p}_2}{(v_1+v_3)}\sqrt{\frac{1}{(v_1+v_3)2\pi}}\exp(-\frac{\mu_3{}^2}{2(v_1+v_3)})\right\}$$

So $\beta = c * \left\{\frac{\mu_2 \mathrm{p}_1}{(v_1+v_2)}\sqrt{\frac{1}{(v_1+v_2)2\pi}}\exp\left(-\frac{\mu_2{}^2}{2(v_1+v_2)}\right) + \frac{\mu_3 \mathrm{p}_2}{(v_1+v_3)}\sqrt{\frac{1}{(v_1+v_3)2\pi}}\exp(-\frac{\mu_3{}^2}{2(v_1+v_3)})\right\}$

Same method for γ

$g''(z) =$

$c * \left\{c_2 \exp\left(-\frac{1}{2}\frac{(z-\mu_2)^2}{v_2}\right)\frac{(z^2+\mu_2{}^2-2\mu_2 z-v_2)}{v_2{}^2} + c_3 \exp\left(-\frac{1}{2}\frac{(z-\mu_3)^2}{v_3}\right)\frac{(z^2+\mu_3{}^2-2\mu_3 z-v_3)}{v_3{}^2}\right\}$

$$\gamma = E\left(g''(z)\right) = (3) + (4)$$

$$(3) = \mathrm{c} * \frac{\mathrm{p}_1\left({\mu_2}^2 - (v_1+v_2)\right)}{\sqrt{2\pi(v_1+v_2)}(v_1+v_2)^2} \exp\left(-\frac{{\mu_2}^2}{2(v_1+v_2)}\right)$$

$$(4) = \mathrm{c} * \frac{\mathrm{p}_2\left({\mu_3}^2 - (v_1+v_3)\right)}{\sqrt{2\pi(v_1+v_3)}(v_1+v_3)^2} \exp\left(-\frac{{\mu_3}^2}{2(v_1+v_3)}\right)$$

$$\gamma = c * \left\{\frac{\mathrm{p}_1\left({\mu_2}^2 - (v_1+v_2)\right)}{\sqrt{2\pi(v_1+v_2)}(v_1+v_2)^2} \exp\left(-\frac{{\mu_2}^2}{2(v_1+v_2)}\right) + \frac{\mathrm{p}_2\left({\mu_3}^2 - (v_1+v_3)\right)}{\sqrt{2\pi(v_1+v_3)}(v_1+v_3)^2} \exp\left(-\frac{{\mu_3}^2}{2(v_1+v_3)}\right)\right\}$$

For g(z) to be the relative fitness function, f(z)g(z) must integrate to one.

$$\int f(z)g(z)dz = 1$$

$$\rightarrow \quad c * \left\{\mathrm{p}_1\sqrt{\frac{1}{2\pi(v_1+v_2)}} \exp\left(-\frac{{\mu_2}^2}{2(v_1+v_2)}\right) + \mathrm{p}_2\sqrt{\frac{1}{2\pi(v_1+v_3)}} \exp\left(-\frac{{\mu_3}^2}{2(v_1+v_3)}\right)\right\} = 1$$

$$c = \left\{\mathrm{p}_1\sqrt{\frac{1}{2\pi(v_1+v_2)}} \exp\left(-\frac{{\mu_2}^2}{2(v_1+v_2)}\right) + \mathrm{p}_2\sqrt{\frac{1}{2\pi(v_1+v_3)}} \exp\left(-\frac{{\mu_3}^2}{2(v_1+v_3)}\right)\right\}^{-1}$$

Here are some examples for bimodal fitness functions and their BQA

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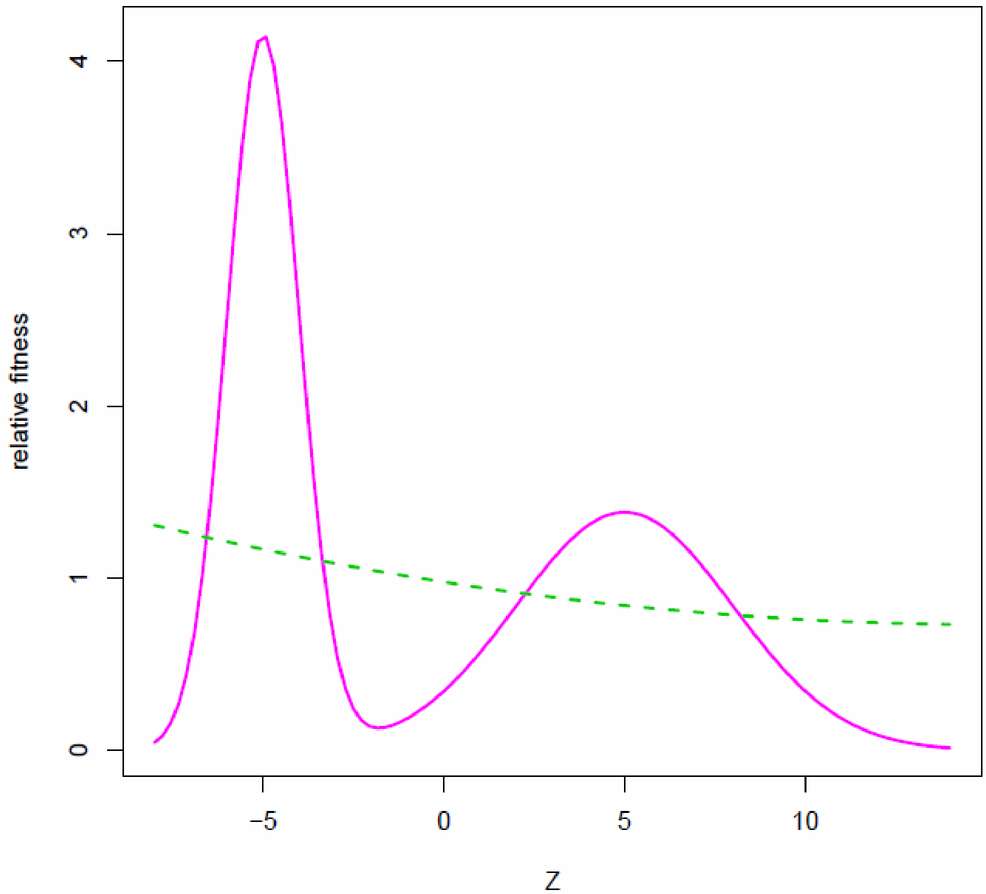
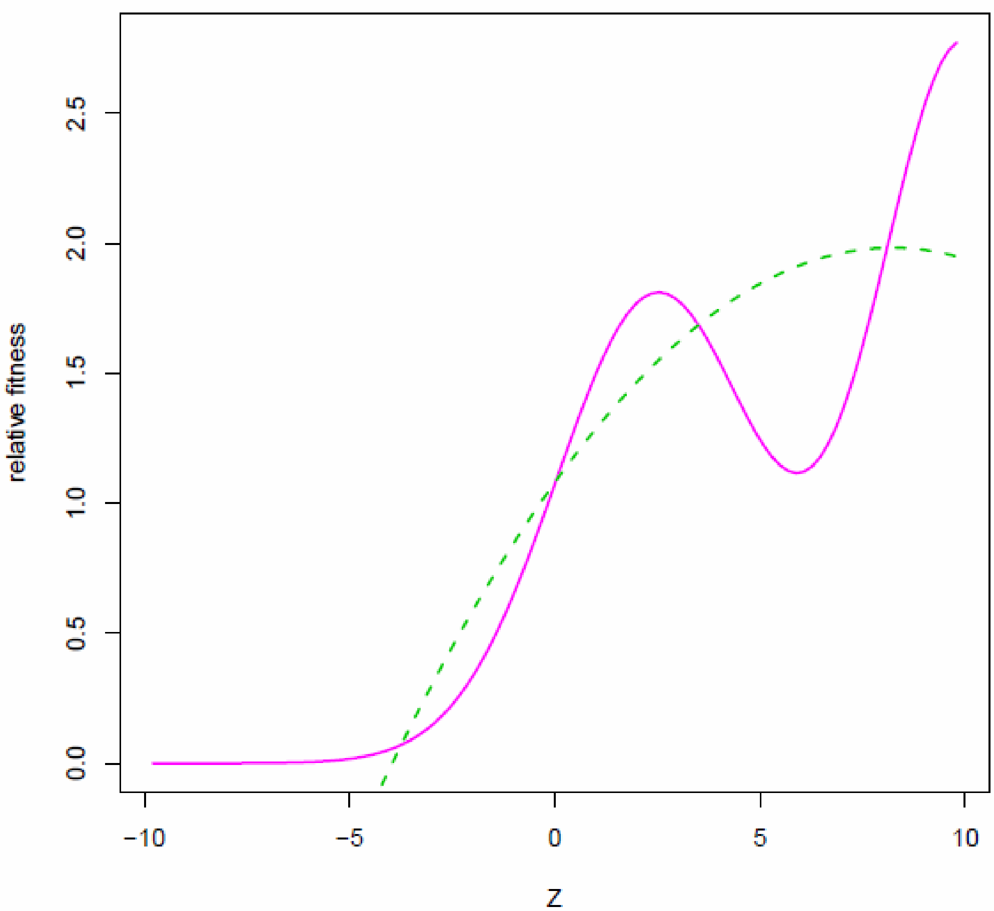

relative fitness
0
1
2
3
4
−5
0
5
10
Z


relative fitness
0.0
0.5
1.0
1.5
2.0
2.5
−10
−5
0
5
10
Z

Reference

1. Charles J. Geyer, Ruth G. Shaw. Commentary on Lande-arnold Analysis. Technical Report No.670. 2008:18-19
2. Charles J. Geyer. Lecture notes. Deck 4, slides 19. <http://www.stat.umn.edu/geyer/5102/slides/s4.pdf>
3. Lande, R. and Arnold, S. J. (1983). The measurement of selection on correlated characters. Evolution, 37, 1210-1226.

R code:

1 unimodal one dimension:

```
v1<-2;

v2<-2;

mu2<-5;

beta<-mu2/(v1+v2)

gamma<-beta^2-1/(v1+v2)

alpha<-1-gamma*v1/2

v3<-1/(1/v1+1/v2)

c2<-sqrt(v1/v3)*exp(mu2^2*(v2-v3)/(2*v2^2))
```

```
zlim<-3

foo<-function(z) alpha+beta*z+gamma*z^2/2

bar<-function(z) c2*exp(-(z-mu2)^2/(2*v2))

zz<-seq(-zlim,zlim,0.01)

ylim<-c(min(foo(zz),bar(zz)),max(foo(zz),

bar(zz)))

curve(foo, col="magenta", ylab="relative fitness",

xlab="Z", from =-3, to =3, ylim=  ylim,lty=2,lwd=2)

curve(bar, col=" green3", add= TRUE, lwd=2)
```

2. bimodal one dimension:

```
v1<-1;v3<-2;v2<-3;mu2<--1;mu3<-5;p1<-0.6;

p2<-1-p1;

a<-p1*sqrt(1/(2*3.14*(v1+v2)))*exp(-mu2^2/(2*(v1+v2)));

b<-p2*sqrt(1/(2*3.14*(v1+v3)))*exp(-mu3^2/(2*(v1+v3)));

c<-1/(a+b)

betap1<-mu2*p1/((v1+v2)*sqrt(2*3.14*(v1+v2)))*exp(-mu2^2/(2*(v1+v2)));

betap2<-mu3*p2/((v1+v3)*sqrt(2*3.14*(v1+v3)))*exp(-mu3^2/(2*(v1+v3)));
```

```
beta<-c*(betap1+betap2);

gammap1<-(mu2^2-v1-v2)*p1/((((v1+v2)^2)*sqrt(2*3.14*(v1+v2)))*exp(-
mu2^2/(2*(v1+v2)));

gammap2<-(mu3^2-v1-v3)*p2/((((v1+v3)^2)*sqrt(2*3.14*(v1+v3)))*exp(-
mu3^2/(2*(v1+v3)));

gamma<-c*(gammap1+gammap2);

alpha<-1-gamma*v1/2;

beta;gamma;alpha;

gf<-function(x){

  y<-c*(p1/sqrt(2*3.14*v2)*exp(-(x-mu2)^2/(2*v2))+p2/sqrt(2*3.14*v3)*exp(-(x-
mu3)^2/(2*v3)));

  return (y);}

g2f<-function(x){

  y<-alpha+beta*x+gamma*x^2/2;

  return (y)}

zlim<-3*sqrt(v1)

zz<-seq(-zlim,zlim,0.01);

ylim<-c(min(gf(zz)),max(gf(zz)));
```

```
curve(gf, col="magenta", ylab="relative fitness",

xlab="Z", from =-zlim, to =zlim, ylim= ylim, lwd=2);

curve(g2f, col=" green3", add= TRUE,lty=2, lwd=2)
```