分子生物计算 (Perl 语言编程)

天津医科大学 生物医学工程与技术学院

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第 10..13 章 GenBank、PDB、BLAST、其他

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- 1 模式匹配
- 2 输入记录分隔符
- ③ 读取文件
- 4 文件夹处理
- 5 格式化输出

- 6 与外部程序进行交互
- 7 浮点数比较
- ⑧ 引用
- 9 模块
- 10 BioPerl

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```
my $name = "manfred";
 2
   if (\text{sname} = \sim / \text{fred}) {
4
        print "You could be fred\n";
 5
   #You could be fred
8
   if (\text{name} = \sim / \text{bfred/b/}) 
9
        print "You ARE fred\n";
10
```



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```
1 if ( $line =~ /^\/\n/ ) {
2    last;
3 }
4    if ( $line =~ m!//\n! ) {
6    last;
7 }
```



```
#!/usr/bin/perl
2
  use warnings;
4
  "AAC\nGTT" =~ /^.*$/;
  print "Without /m:\n", $&, "\n";
  #Without /m:
8 #Use of uninitialized value $& in print at
    XXX.pl line N.
9
10 "AAC\nGTT" =~ /^.*$/m;
11 print "With /m:\n", $&, "\n";
12 | #With /m:
13 #AAC
```

```
#!/usr/bin/perl
2
  use warnings;
4
  "AAC\nGTT" =~ /^.*$/;
6 print "Without /s:\n", $&, "\n";
  #Without /s:
8 #Use of uninitialized value $& in print at
    XXX.pl line N.
9
10 "AAC\nGTT" =~ /^.*$/s;
11 print "With /s:\n", $&, "\n";
12 #With /s:
13 # AAC
14 #GTT
```

模式匹配 | 捕获

```
1 #!/usr/bin/perl
2
  use strict; use warnings;
4
5 my $alphabet = join "", 'a' .. 'z';
6 |$alphabet =~ /k(lmnop)q/;
7|print $1, "\n\n";
8 #lmnop
9
10 | alphabet = ~ /(((a)b)c)/;
11|print "First pattern = ", $1, "\n";
12 print "Second pattern = ", $2, "\n";
13 print "Third pattern = ", $3, "\n";
14 #First pattern = abc
15 #Second pattern = ab
16 #Third pattern = a
```



```
my $string = "File code=123 name=test.txt";
 | if (\$string = \ /code = (\d+) \s+name = ([\w\.]+)/)  {
3
     print "Code is $1\nName is '$2'\n";
4
```

```
my %q count;
 while (<>) {
     while (/\b(Q\w+)\b/q) {
4
          ++$q count{$1};
5
6
 foreach my $word (sort {$q count{$b}<=>$q count{$a
   }} keys %q count) {
8
     print "The word $word appeared ",$q count{
   $word}," times\n";
9
```



模式匹配 | 正则表达式

When not to use Regular Expressions

- Splitting delimited data: split
- Swapping single characters: tr
- Extracting fixed position data: substr
- Finding the position of an exact string: index





```
my $string = "xxxxxxhixxxxxxxxhixxxxxxxhi";
 my $lastpos = 0;
3
 while (1) {
5
     my $pos = index($string, "hi", $lastpos);
6
     last if ($pos == -1); # Substring not
   found
     print "Found hi at index $pos\n";
8
     1 = ++ pos;
9
```



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输入记录分隔符

```
1 my $save_input_separator = $/;
2
3 $/ = "//\n";
4 $record = <GBFILE>;
5
6 $/ = $save_input_separator;
```



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```
for (;;) {
    for ($curpos = tell(FILE); $_ = <FILE>;
    $curpos = tell(FILE)) {
        # search for some stuff and put it
    into files
4    }
    sleep($for_a_while);
    seek(FILE, $curpos, 0);
}
```



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文件夹处理 | 递归

```
1 #!/usr/bin/perl
2 use strict; use warnings;
3 list recursively('pdb');
  sub list recursively {
      my ($directory) = 0;
      mv @files = ();
      unless ( opendir ( DIRECTORY, $directory ) ) {
           print "Cannot open directory $directory!\n";
10
          exit:
11
12
      @files = grep ( !/^\.\.?$/, readdir(DIRECTORY) );
      closedir(DIRECTORY);
13
14
      foreach my $file (@files) {
           if ( -f "$directory/$file" ) {
15
16
               print "$directory/$file\n";
17
18
           elsif ( -d "$directory/$file" ) {
               list recursively("$directory/$file");
19
20
21
22
```



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文件夹处理 | 模块

```
#!/usr/bin/perl
2
3 use strict;
4 use warnings;
5 use File::Find;
6 #perldoc File::Find
7
  find( \&my sub, ('pdb') );
9
10
  sub my sub {
11
      -f and ( print $File::Find::name, "\n" );
12
```



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文件夹处理 | 通配

```
# <*>
2 | my  @files = <*.doc>;
  print "I have ", scalar @files," doc files in
   my work directory\n";
4
5 # glob
  my @files2 = glob("*.rtf");
  print "I have ", scalar @files2," rtf files in
     my work directory\n";
8
  chdir ("/home") or die "Can't move to work
    directory: $!";
  while (my file = <*.doc>) {
10
11
      print "Found file $file\n";
12
```



文件夹处理 | 定位

```
1 #!/usr/bin/perl
  use warnings; use strict;
3
  # If you want to open a file in a location
    relative to the location of your script
    then you can use the FindBin module to get
    the filesystem location of your Perl
    program.
  use FindBin qw($Bin);
6
  # This code will add the ExtraModules
    directory to the module search path.
  use lib "$Bin/ExtraModules";
9
10 print "Script is located in $Bin\n";
```

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```
while (<>) {
2
    /^ATOM/ or next;
3
4
    my($n, $x, $y, $z, $element)
5
       = (\$ = ^{.}\{6\} (.\{5\}).\{19\} (.\{8\}) (.\{8\})
     (.{8}).{22}(..)/);
6
     =\sim s/^{s}/s*//;
8
     ext{$element =~ s/^s*//}
9
10
    if ((\$n == 1) \text{ or } (\$n == 1078))
11
       printf "%8.3f%8.3f%8.3f %2s\n", $x, $y,
    $z, $element;
12
13
```

格式化输出 | printf

```
my $first = '3.14159265';
my $second = 76;
my $third = "Hello world!";

printf STDOUT "A float: %6.4f An integer: %-5
   d and a string: %s\n", $first, $second,
   $third;

#A float: 3.1416 An integer: 76 and a
   string: Hello world!
```



```
1 #!/usr/bin/perl
2 use strict; use warnings;
  my $DNA = 'AAACCCCCGGGGGGGGTTTTTT';
  for (my \$i = 0; \$i < 2; ++\$i) {
5
      print <<HEREDOC;</pre>
6
       On iteration $i of the loop!
      $DNA
8
  HEREDOC
10
11
        On iteration 0 of the loop!
12
       AAACCCCCGGGGGGGGTTTTTT
13
14
        On iteration 1 of the loop!
15
       AAACCCCCGGGGGGGGTTTTTT
16
```

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```
1 #!/usr/bin/perl
2 use strict; use warnings;
3 my $id
         = 'A0000';
4 my $description = 'Highly weird DNA. This DNA is so
  unlikelv!';
5 \text{ my } \text{$DNA = '}
   6 # Define the format
7 format STDOUT =
8 # The header line
9|>@<<<<<< @<<<<<<<...
10 $id, $description
11 # The DNA lines
12| ^<<<<<<<<<<<<<<<<<<<<<<<<
13 SDNA
14
15 # Print the fasta-formatted DNA output
16 write;
```

格式化输出 | format & write

```
>A00000 Highly weird DNA. This DNA is so un...
```

3 TTTTTTTTTTTTT



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外部程序 | 运行 | 简介

用途

Using the functions described in this next slide it is straightforward to either pass data through an external program as part of your Perl script, use Perl as a glue language to automate the execution of other programs, or simply use Perl as a convenient way to launch anther program.

三种方法

There are three different functions you can use within Perl to launch an external program. These are <code>system</code>, backticks (` `) and <code>exec</code> and they all have slightly different purposes.



外部程序 | 运行 | 简介

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三种方法

There are three different functions you can use within Perl to launch an external program. These are system, backticks (` `) and exec and they all have slightly different purposes.



外部程序 | 运行 | 方法

system

System is used where you want to launch an external program and check that it worked, but you don't need to collect any data back from it.

backticks

If you want to get hold of the output of programs then you need to use backticks rather than system.

exec

Exec is a somewhat unusual function in perl as it causes execution of your perl program to end immediately, and your running perl program is replaced by whatever program you specify.



外部程序 | 运行 | 方法

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```
1 | my  $filename = $ARGV[0];
2 my $stride = '/usr/local/bin/stride';
 3 | mv  $options = '';
4 # 捕获输出
5 my @results = `$stride $options $filename`;
6 | mv  $now = `date`;
 7|_{\text{my}} @functions = qw( int rand length );
8 my %about;
9 foreach (@functions) {
10  #$about{$ } = `perldoc -t -f $ `;
11 | about\{ \} = qx(perldoc -t -f \} );
12|}
13
14 # 不捕获输出, 返回值为程序退出状态
15 system "$stride $options $filename";
16 system 'date';
17 system 'tar', 'cvf', $tarfile, @dirs;
```



外部程序|管道|接入

Piping data out of an external program

```
1 open (my $log, "tail -f /var/log/httpd/
  access_log |") or die "Can't open pipe to
  web logs: $!";
2
3 while (<$log>) {
   if (/Safari/) {
      print "Oooh, a Mac user...\n";
   }
7 }
```



外部程序 | 管道 | 导出

Piping data into an external program

```
1 open (my $zip, "| zip compress.zip -") or die
    "Can't open pipe to zip: $!";
2
3 print $zip "I want to be smaller...";
4
5 close $zip or die "Can't close pipe to zip:
    $!";
```



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浮点数比较

```
1 #!/usr/bin/perl
2
  if (10 / 3 == ((1 / 3) * 10)) {
4
     print "Success!\n";
5
  else { print "Failure!\n"; }
7
  #Failure!
8
9 \mid \text{if } (abs(10/3 - ((1/3) * 10)) < 1e-10) 
10
    print "Right!\n";
11
     print "E=", abs(10/3 - ((1/3) * 10)), "\n";
12 }
13 else { print "Wrong!\n"; }
14 #Right!
15 #E=4.44089209850063e-16
```

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引用 | 匿名

```
my @array = (1, 2, 3, 4);
  my $slow arrayref = \@array;
  my quick arrayref = [1, 2, 3, 4];
4
  my %hash = (
6
     dog => 'woof',
      cat => 'meow',
8
  );
  my $slow hashref = \%hash;
10 my $quick hashref = {
11
     dog => 'woof',
12
      cat => 'meow',
13 };
```

```
my $arrayref = [10, 20, 30];
 print "First element is ", $$arrayref[0],
   n";
3 print "First element is ", $arrayref->[0],
   n";
4
 my $hashref = {
6
    duck => 'quack',
 };
 print "The duck says ", $$hashref{duck},
                                             "\n
9 print "The duck says ", $hashref->{duck}, "\n
   ";
```

引用 | 拷贝

```
1|_{my} @original = (2, 4, 6, 8);
2 my @copy = @original;
3 for (0..$#copy) { $copy[$ ] *= 10; }
4 print "Copy says ", $copy[1], " but original
    was ",$original[1];
5 # The copy is altered so the second element
    is 40, but the original still says 4.
6
7|_{\text{my}} $original = [2, 4, 6, 8];
8 my $copy = $original;
9 | for (0..(@$copy-1)) { $copy->[$ ] *= 10; }
10 print "Copy says ", $copy->[1]," but original
    was ",$original->[1];
11 # Both the original and copy references point
     to an array whose second element is 40.
```



Country	Population	Language	Currency
UK	60,441,457	English	Pounds
France	60,656,178	French	Euros
Ireland	4,015,676	English/Irish	Euros



```
my %countries;
2 | my %uk info = (
3
     population \Rightarrow 60441457,
4
      language => 'English',
5
     currency => 'Pounds',
6);
7|_{\text{my}} %france info = (
8
       population => 60656178, language => 'French',
    currency => 'Euros',
9);
10 | my  %ireland info = ( ... );
11
12 \countries\{uk\} = \c info;
13 | $countries {france} = \%france info;
14 | #$countries{ireland} = \%ireland info;
15
16 print "Population of France is ",
17
       $countries{france}->{population},"\n";
```



```
my %countries = (
2
       uk => {
3
           population \Rightarrow 60441457,
4
           language => 'English',
5
            currency => 'Pounds',
6
7
       },
       france => {
8
           population => 60656178,
9
            language => 'French',
10
           currency => 'Euros',
11
       },
12
       ireland => {
13
14
       },
15);
16
  print "Population of France is ",
18
       $countries{france}->{population}, "\n";
```



```
1 my %countries;
2
3 $countries{uk} -> {population} = 60441457;
4 $countries{france} -> {population} = 60656178;
5 $countries{france} -> {currency} = 'Euros';
6
7 print "Population of France is ",
8 $countries{france}->{population},"\n";
```



Data: country.txt

Task

Q: Population of France

A: 60,656,178



Data: country.txt

Task

Q: Population of France

A: 60,656,178



shell

```
1 grep -i -w France country.txt | cut -f2
```

csvkit

- 1 # Method 1
- 2 csvsql --query "select Population from country where Country=='France'" country. txt | csvlook
- 3 # Method 2
- 4 csvgrep -t -c Country -m France country.txt | csvcut -c Population | csvlook

shell

```
1 grep -i -w France country.txt | cut -f2
```

csvkit

- csvsql --query "select Population from country where Country=='France'" country. txt | csvlook
- 3 # Method 2

1 # Method 1

4 csvgrep -t -c Country -m France country.txt | csvcut -c Population | csvlook

Perl-hash

```
1 #!/usr/bin/perl
2 use strict; use warnings;
3 my $fi = "country.txt";
4 my (@header, @fields, %countries);
5 open my $IN, '<', $fi or die "$0 : failed to open input file '
    $fi': $!\n";
  while (<$IN>) {
      chomp:
8
      if ($. == 1) {
9
           @header = map { lc } split /\t/;
10
11
       else {
12
           @fields = map { lc } split /\t/;
13
           for ( mv $i = 1 ; $i < @header ; $i++ ) {
14
               $countries{$fields[0]}->{$header[$i]}=$fields[$i];
15
16
17
18 close $IN or warn "$0: failed to close input file '$fi': $!\n";
19 print "Population of France is ", $countries{france}->{
    population}, "\n";
```

Perl-Data::Table

```
1 #!/usr/bin/perl
2
  use strict:
4 use warnings;
5 use Data::Table;
6
  my $countries = Data::Table::fromFile("country.txt
    ");
8
  print "Population of France is ",
10
    $countries->
11
    match pattern hash('$ {Country} eq "France"')->
12
    col('Population'),
13
    "\n";
```

```
R
```

```
1 library(readr)
2 library(dplyr)
3
4 countries <- read_tsv("country.txt")
countries %>%
6 filter(Country=="France") %>%
7 select(Population)
```



```
@experiments = (
2
3
            sample id \Rightarrow 1,
4
            sample name => 'kidney',
5
            sample measures \Rightarrow [12,56,34,65,76],
6
       },
 7
8
            sample id \Rightarrow 4,
9
            sample name => 'liver',
10
            sample measures \Rightarrow [24,66,12,17,26],
11
12
        { ... },
13);
14
15 foreach my $expt (@experiments) {
16
       print "The first measure for sample ",
17
              $expt->{sample id},
18
               " (", $expt->{sample name}, ") was ",
19
              $expt->{sample measures}->[0],"\n";
20
```



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```
#METHOD 1: cpan
  #Open cpan shell
  sudo cpan
4 # or
  perl -MCPAN -e shell
6 #Install modules
  cpan>install Date::Calc
8
9 # METHOD 2: cpanm
10 #Install cpanm
11 perlbrew install-cpanm
12 #Install modules
13 cpanm Bio::Perl
14
15
  # METHOD 3: manual
16
```



```
#!/usr/bin/perl
2
3 use warnings;
4 use strict;
5
 use Date::Calc qw(:all);
 #use Date::Calc qw(Days in Year Days in Month
   ) ;
8
 print "In Feb 2020 there are ", Days in Month
    (2020,2)," days";
```



```
1 #!/usr/bin/perl
2
  use warnings; use strict;
4
5 use LWP::UserAgent;
6
  my $ua = LWP::UserAgent->new;
8 $ua->timeout(10);
9 $ua->env proxy;
10
  my $response=$ua->get('http://search.cpan.org/');
12
13 if ($response->is success)
14
      print $response->decoded content;
15 }
16 | else {
17
      die $response->status line;
18|}
```



模块 | 编写 | 函数式编程

```
#!/usr/bin/perl
2
  use warnings;
  use strict;
5
  package Example::Module;
8
  # Module code goes here
9
10
```



```
#!/usr/bin/perl
  use warnings; use strict;
  use Exporter;
  our @ISA = qw(Exporter);
  our @EXPORT OK = qw (will be exported);
   sub public {
       # This is designed to be seen, but can only be addressed by
    using its fully qualified name eq Example::Functional::public
10
  sub private {
      # This is only for internal use and shouldn't be used from
    outside the module.
13
14 sub will be exported {
15
       # This can be exported into the namespace of the calling
16
17
18 1;
```



模块 | 编写 | 面向对象编程(1/2)

```
1 #!/usr/bin/perl
2
  use warnings;
  use strict;
5
  package Example::Object oriented;
  sub new {
      # This creates the reference which is going to be
    our object
10
      my $hashref = {};
11
      # We then call bless to associate it with this
    module.
12
      bless Shashref:
13
      # Finally we return it so the calling program can
    start using it.
      return $hashref:
14
15
```



```
16 sub save value {
17
    # This subroutine takes a single arguement which it
    stores in the hash reference. The $object is provided
    automatically as the first argument to every object
    oriented subroutine (other than 'new').
18
      my ($object, $new value) = @ ;
19
      $object->{value} = $new value;
20 }
21
  sub get value {
22
      # This subroutine retrieves a value which was
    previously stored via the save value subroutine. If
    there isn't a value to retrieve it returns the
    undefined value.
23
      my ($object) = 0;
24
      if (exists $object->{value}) {return $object->{value}
    };}
25
     else { return undef; }
26
27
28 1;
```

模块 | 编写 | 面向对象编程 | 使用

```
#!/usr/bin/perl
2
  use warnings;
4 use strict:
5
  use Example::Object oriented;
7
  my $object = Example::Object oriented->new();
9
10
  $object->save value("Hello");
11
12 print "The object says '". $object->get value
    () . "'\n";
```

教学提纲

- 1 模式匹配
- 2 输入记录分隔符
- ③ 读取文件
- 4 文件夹处理
- 6 格式化输出

- 6 与外部程序进行交互
- 7 浮点数比较
- ③ 引用
- 9 模块
- 10 BioPerl



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```
use Bio::SeqIO;
2
  my $string = ">SEQ1\nacgt\n>revseq1\ntgca ";
  my $format = "fasta";
5
  my $stringfh = IO::String->new($string);
  open($stringfh, "<", $string) or die "Could not open
    string for reading: $!";
8
  my $segio = Bio::SegIO-> new(-fh => $stringfh,
10
                                -format => $format.
11
                               );
12
13 while ( my $seq = $seqio->next seq ) {
14
     print $seq->id . ' = ' . $seq->seq() . "\n";
15
```

```
1 use strict; use Bio::SeqIO;
2 my $input file = shift;
3 my $seq in = Bio::SeqIO->new( -format => 'embl',
4
                                   -file => $input file,
5
                                  );
6 my @seq array;
7 while ( my $seq = $seq in->next_seq() ) {
8
    push (@seq array, $seq);
10 @seq array = sort { $a->length <=> $b->length }
    @seq array;
11 \mid my $total = 0;
12 \text{ my } \text{ $count = 0;}
13 for my $seq (@seq array) {
$\text{$total += $seq->length;}
15
   $count++;
16 }
17 print "Mean length ", $total/$count, " Median ",
18
         $seq array[$count/2]->length, "\n";
```



```
use Bio::SeqIO;
 2
  my $usage = "x2y.pl infile informat outfile outformat";
4 my $infile = shift or die $usage;
5 my $informat = shift or die $usage;
 6 my $outfile = shift or die $usage;
  my $outformat = shift or die $usage;
8
  my $seq in = Bio::SeqIO->new( -file => "$infile",
10
                                 -format => $informat,
11
  my $seq out = Bio::SeqIO->new( -file => ">$outfile",
13
                                  -format => $outformat,
14
15 while (my $inseq = $seq in->next seq) {
16
     $seq out->write seq($inseq);
17
```

```
use Bio::SeqIO;
   my $usage = "splitgb.pl infile "; my $infile = shift or die $usage;
   my $inseq = Bio::SeqIO->new( -file => "<$infile", -format => 'Genbank',);
   my %outfiles = ( human => {
5
6
7
8
9
10
                            Genbank => Bio::SegIO->new(
                                                         -file => '>human.gb',
                                                         -format => 'Genbank',
                             Fasta => Bio::SegIO->new(
                                                         -file => '>human.fa',
11
                                                         -format => 'Fasta'.
12
13
14
                    other =>
15
                             Genbank => Bio::SegIO->new(
16
                                                         -file => '>other.gb',
17
                                                         -format => 'Genbank',),
18
                             Fasta => Bio::SegIO->new(
19
                                                         -file => '>other.fa',
20
                                                         -format => 'Fasta',),
21
22
                  );
23
   while (my $seqin = $inseq->next seq)
      if ($segin->species->binomial =~ m/Homo sapiens/)
24
25
          $outfiles{'human'}->{'Genbank'}->write seq($seqin);
26
          $outfiles('human')->{'Fasta'}->write seq($seqin);
27
      } else {
28
          $outfiles{'other'}->{'Genbank'}->write seg($segin);
29
          $outfiles{'other'}->{'Fasta'}->write seq($seqin);
30
31
```



```
use Bio::DB::GenBank;
2 use Bio::DB::Query::GenBank;
3
  $query = "Arabidopsis[ORGN] AND topoisomerase[TITL] and
    0:3000[SLEN]";
5 | $query obj = Bio::DB::Query::GenBank->new(-db => '
    nucleotide',
6
                                              -query =>
    $query );
 7
  $gb obj = Bio::DB::GenBank->new;
9
  $stream obj = $qb obj->qet Stream by query($query obj);
11
12 while ($seq obj = $stream obj->next seq) {
13
       # do something with the sequence object
14
      print $seq obj->display id, "\t", $seq obj->length,
    "\n";
15 }
```



```
1 #!/usr/bin/perl
2 use strict; use warnings;
3 use Bio::DB::Query::GenBank; use Bio::DB::GenBank;
4 use Bio::SeqIO;
6 my $query string = $ARGV[0];
7 my $fo fa=$query string.".fa"; my $fo gb=$query string.".gb";
8 my $query = Bio::DB::Query::GenBank->new(
      -db => 'nucleotide', -query => $query string
10 );
11 my $qb = Bio::DB::GenBank->new;
12 my $stream = $gb->get Stream by query($query);
13
14 my %outfiles = (
    Fasta => Bio::SeqIO->new( -file => ">$fo fa", -format => '
15
   Fasta',),
      Genbank => Bio::SeqIO->new( -file => ">$fo qb", -format => '
16
    Genbank',),
17 );
18 while ( my $seq = $stream->next seq ) {
      $outfiles{'Fasta'}->write seq($seq);
19
      $outfiles{'Genbank'}->write seg($seg);
20
21
```

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