# 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

> 2018-2019 学年上学期(秋) 2016 级生信班

#### 第 10..13 章 GenBank、PDB、BLAST、其他

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2019年1月





- 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
 7
8
   if (\text{name} = \sim / \text{bfred/b/}) 
9
        print "You ARE fred\n";
10
```



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



```
#!/usr/bin/perl
2
  use warnings;
4
5 "AAC\nGTT" =~ /^.*$/;
6 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
5 "AAC\nGTT" =~ /^.*$/;
6 print "Without /s:\n", $&, "\n";
7 #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
```

```
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 #1mnop
9
10 = (((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
```



#### 模式匹配 | 捕获

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

```
1 my %q_count;
2 while (<>) {
      while (/\b(Q\w+)\b/g) {
          ++$q_count{$1};
      }
6 }
7 foreach my $word (sort {$q_count{$b}<=>$q_count{$a}} keys %q_count) {
      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
7
     print "Found hi at index $pos\n";
8
     $lastpos = ++$pos;
9
```



- 输入记录分隔符





### 输入记录分隔符

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



- 读取文件





```
for (;;) {
    for ($curpos = tell(FILE); $_ = <FILE>;
    $curpos = tell(FILE)) {
        # search for some stuff and put it
    into files
}
sleep($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;
  list recursively('pdb');
  sub list recursively {
      my ($directory) = 0;
      mv @files = ();
8
      unless ( opendir ( DIRECTORY, $directory ) ) {
           print "Cannot open directory $directory!\n";
          exit:
10
11
      @files = grep ( !/^\.\.?$/, readdir(DIRECTORY) );
12
13
      closedir(DIRECTORY);
      foreach my $file (@files) {
14
           if ( -f "$directorv/$file" ) {
15
               print "$directory/$file\n";
16
17
           elsif ( -d "$directory/$file" ) {
18
19
               list recursively("$directory/$file");
20
21
22
```

### 文件夹处理 | 模块

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



### 文件夹处理 | 通配

```
# <*>
  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: $!";
10 while (my file = \langle *.doc \rangle) {
11
      print "Found file $file\n";
12
```



### 文件夹处理 | 定位

```
#!/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
```



### 格式化输出 | format & write

```
1 #!/usr/bin/perl
2 use strict; use warnings;
3 my $id
       = 'A0000';
4 my $description = 'Highly weird DNA. This DNA is so
  unlikely!';
5 \text{ my } \$DNA = '
  6 # Define the format
7 format STDOUT =
8 # The header line
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

```
1 >A0000 Highly weird DNA. This DNA is so un...
```

3 TTTTTTTTTTTT



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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.



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# 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.



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#### 外部程序 | 运行 | 举例

```
1 | my  $filename = $ARGV[0];
2 my $stride = '/usr/local/bin/stride';
3 my $options = '';
4 # 捕获输出
5 my @results = `$stride $options $filename`;
6 | my  $now = `date`;
7|my @functions = qw( int rand length );
8 my %about;
9 foreach (@functions) {
10 \#$about{$ } = `perldoc -t -f $ `;
11 \Rightarrow \text{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 }
```



#### 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
6|else { print "Failure!\n"; }
  #Failure!
8
9 | \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);
2 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];
2 print "First element is ", $$arrayref[0],
   n";
 print "First element is ", $arrayref->[0],
   n";
4
 my $hashref = {
6
     duck => 'quack',
 };
 print "The duck says ", $$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|_{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



```
1 my %countries;
2|_{\text{my}} %uk info = (
3
    population => 60441457,
4
      language => 'English',
5
      currency => 'Pounds',
6);
  my %france info = (
8
     population => 60656178, language => 'French',
    currency => 'Euros',
9);
10 | my  %ireland info = ( ... );
11
12 | $countries {uk} = \%uk 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
3
       11k => {
           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
17
  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

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

# 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>) {
7
       chomp;
8
       if ($. == 1) {
9
          @header = map { lc } split /\t/;
10
11
       else {
12
           @fields = map { lc } split /\t/;
13
           for ( my \ \$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")
5 countries %>%
6 filter(Country=="France") %>%
7 select(Population)
```



```
my @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 => [24,66,12,17,26],
11
       },
12
13);
14
   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
```



# 教学提纲

- 模块





```
#METHOD 1: cpan
2 #Open cpan shell
  sudo cpan
4 #or
5 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
 use warnings;
4 use strict;
5
6 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
  1;
```



## 模块 | 编写 | 函数式编程

```
1 #!/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
11
  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)

```
#!/usr/bin/perl
2
  use warnings;
  use strict;
5
  package Example::Object oriented;
7
  sub new {
9
      # 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.
14
      return $hashref;
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;
```



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

# 教学提纲

- **BioPerl**





```
use Bio::SeqIO;
2
  my $string = ">SEQ1\nacgt\n>revseq1\ntgca ";
  my $format = "fasta";
5
6 my $stringfh = IO::String->new($string);
  open ($stringfh, "<", $string) or die "Could not open
    string for reading: $!";
8
  my $seqio = Bio::SeqIO-> new(-fh => $stringfh,
10
                                -format => $format,
11
                               );
12
13 while ( my $seq = $seqio->next seq ) {
     print $seq->id . ' = ' . $seq->seq() . "\n";
14
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);
9
10 @seg array = sort { $a->length <=> $b->length }
    @seq array;
11 | mv  $total = 0;
12 \text{ my } \text{ $count = 0;}
13 for my $seq (@seq array) {
14
     $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
12
  my $seq out = Bio::SeqIO->new( -file => ">$outfile",
                                  -format => $outformat,
13
14
                                );
15 while (my $inseq = $seq in->next seq) {
16
     $seq out->write seq($inseq);
17
```

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



```
1 use Bio::DB::GenBank;
  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
8
  $gb obj = Bio::DB::GenBank->new;
9
  $stream obj = $gb obj->get Stream by query($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 $fo qb=$query string.".qb";
8 my $query = Bio::DB::Query::GenBank->new(
     -db => 'nucleotide', -query => $query string
10 );
11 my $qb = Bio::DB::GenBank->new;
12 my $stream = $qb->qet Stream by query($query);
13
14 my %outfiles = (
15
    Fasta => Bio::SeqIO->new( -file => ">$fo fa", -format => '
   Fasta',),
      Genbank => Bio::SeqIO->new( -file => ">$fo qb", -format => '
16
   Genbank',),
17 );
18 while ( my $seg = $stream->next seg ) {
19
      $outfiles{'Fasta'}->write seq($seq);
      $outfiles{'Genbank'}->write seq($seq);
20
21
```



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