Monte Carlo Integration

Biostatistics 615/815
Lecture 22

Reminders

- No lecture on Thursday, November 30
- Project due on by December 8
  - Short descriptive report (about 2 pages)
  - Code and instructions on how to use it
- Review session on December 7
- Midterm on December 12

Midterm Topics

- Random number generation
- Numerical optimization
  - Golden search
  - Parabolic interpolation
  - Nelder Mead simplex method
  - Simulated annealing
  - Gibbs sampler
- Numerical Integration
  - Classical methods
  - Monte-Carlo integration

Last Lecture …

- Numerical integration
- Classical strategies, with equally spaced abscissas
- Discussion of quadrature methods and Monte-Carlo methods

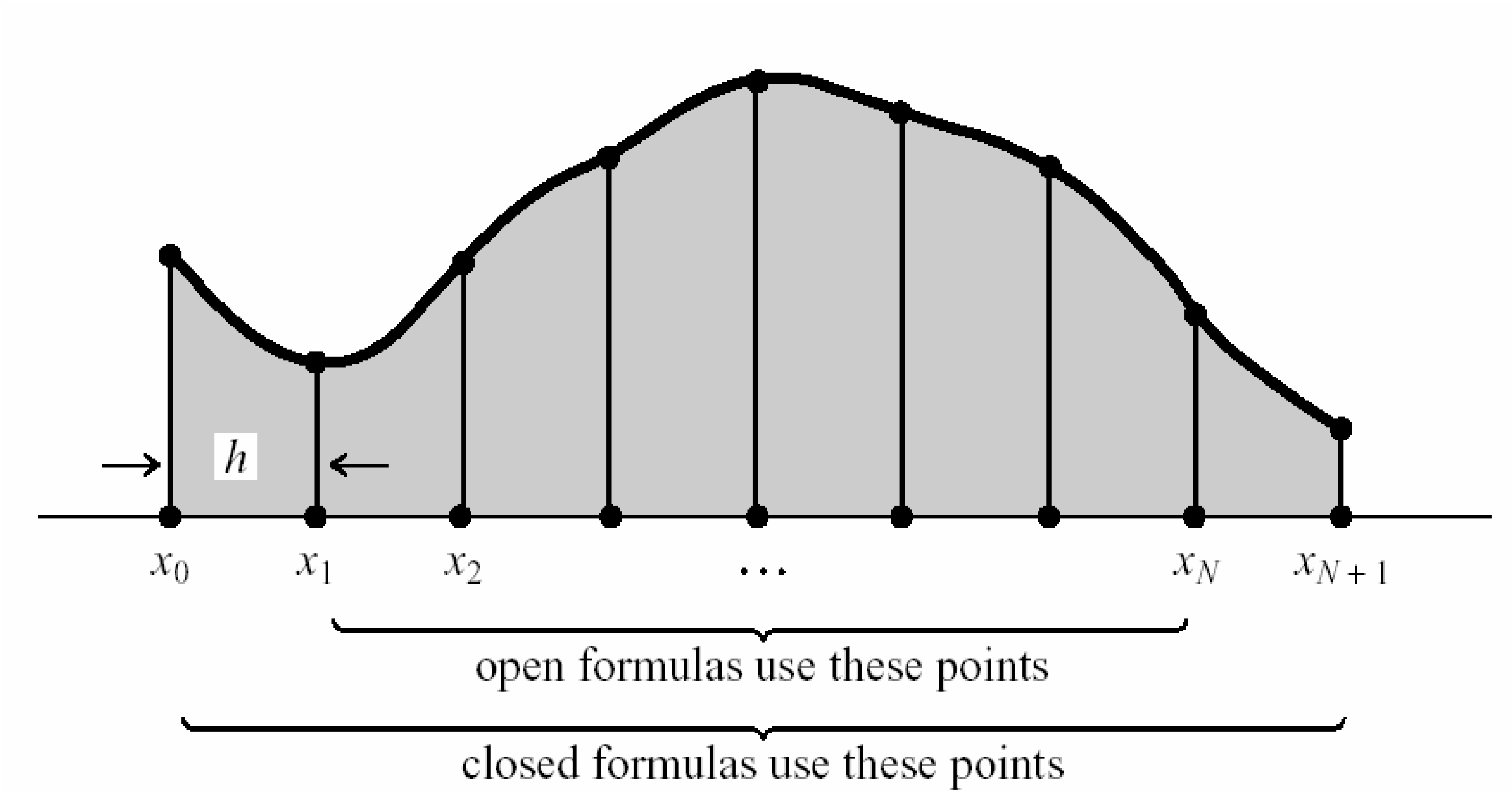
The Problem

- Evaluate:

$$I = \int_a^b f(x)dx$$

- When no analytical solution is readily available
- Evaluate $f(x)$ as few times as necessary
- Things to consider:
  - The choice of abscissas
  - The choice of weights for combining results

The Basic Approach



Classical Solutions

- Trapezoidal Rule
- Simpson's rule

- Adaptive integration
  - Doubled the number of points at each round…

- Gaussian quadrature methods
  - Improved accuracy for smooth functions

Today: Monte Carlo Integration

Basic Monte Carlo Integration

- Consider a multidimensional volume V
- Consider N random points within V
  - $x_1, x_2, \ldots x_N$
- Evaluate the function f at each point …
- … use observed average to estimate integral

Definitions

- The average function value

$$\langle f \rangle \equiv \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

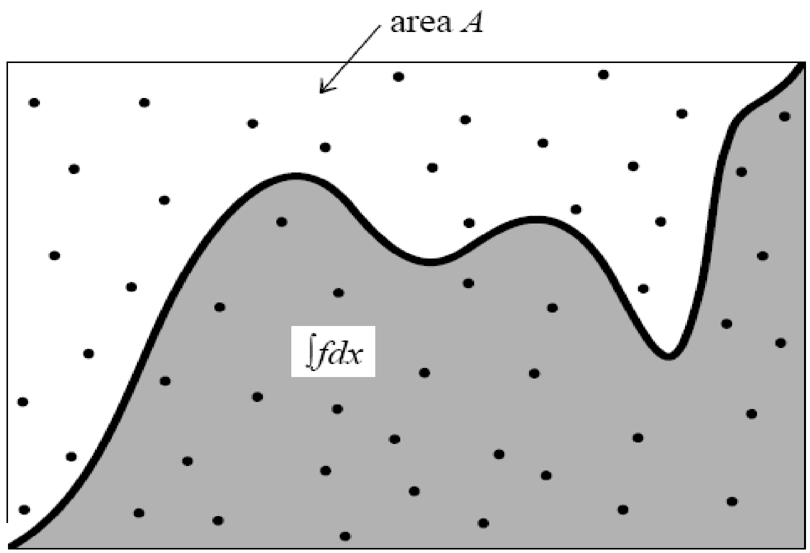
- The average squared function value

$$\langle f^2 \rangle \equiv \frac{1}{N} \sum_{i=1}^{N} f^2(x_i)$$

- Estimate of the integrand (+/- standard error)

$$\int f \, dV \approx V \langle f \rangle \pm V \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}}$$

Simple Monte Carlo Integration



- Sample points within A
- Calculate proportion π of points in region of interest
- Area under the curve is the area A π

C Code: Sampling a Point

```
// This code assumes the Random() function returns a
// uniformly distributed random number between zero and
// one. It then samples a random point within a
// multidimensional “rectangular” space.

void SamplePoint(double * point, double * lo, double * hi,
                int dim)
   {
   for (int i = 0; i < dim; i++)
      point[i] = lo[i] + Random() * (hi[i] - lo[i]);
   }
```

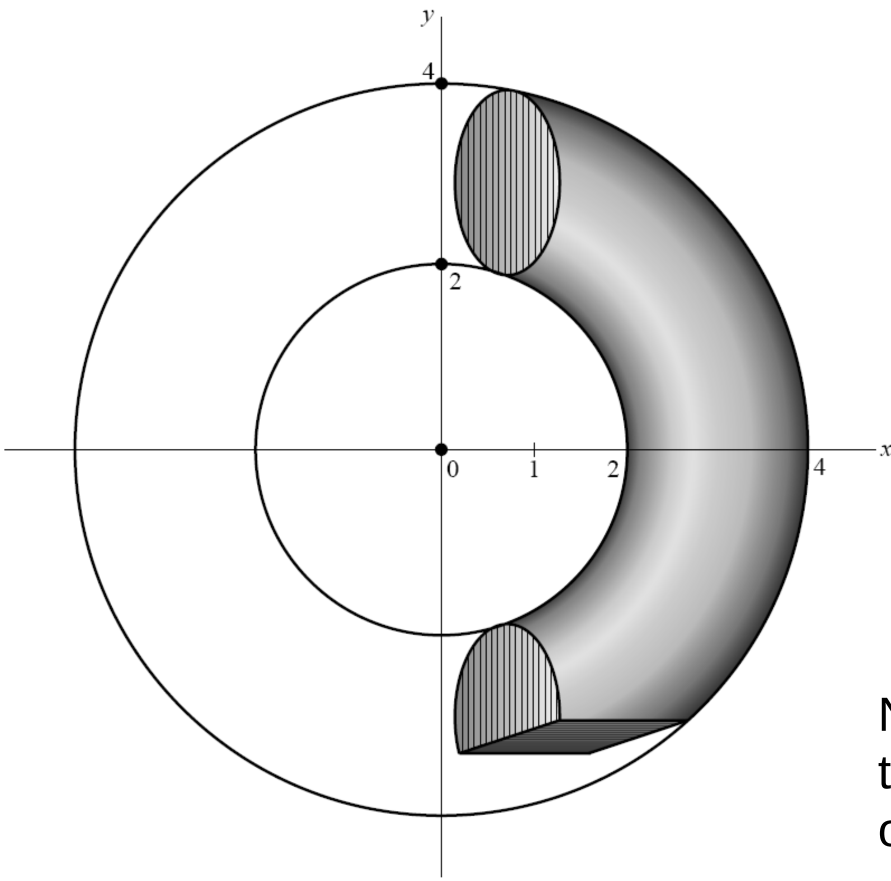
C Code: Monte Carlo Integral

```
double Integrate(double (*f)(double *, int),
                 double * lo, double * hi, int dim, double N)
   {
   double * point = alloc_vector(dim);
   double sum = 0.0, sumsq = 0.0;

   for (int i = 0; i < N; i++)
      {
      SamplePoint(point, lo, hi, dim);

      double fx = f(point, dim);
      sum += fx;
      sumsq += fx * fx;
      }

   double volume = 1.0;
   for (int i = 0; i < dim; i++)
      volume *= (hi[i] - lo[i]);

   free_vector(point, dim);
   return volume * sum / N;
   }
```

Sampling Points

- We saw how to sample points from a simple “rectangular” region …
- … what if the region of interest as a complicated shape?
- Do you have any ideas?

A Complicated Target Region



Numerical Recipes uses this volume as an example of Monte Carlo integration.

The Error Term ...

- In simple Monte-Carlo integration the error term decreases with $\sqrt{N}$
- This is not quite as good as with our classic formulas which used equally spaced points…
  - In those formulas, error is generally proportional to 1/N

Challenge

- Flexibility of Monte Carlo integration …
  - Easy to add more points as needed
- Efficiency of solutions based on equally spaced points
  - Accuracy increases faster than $\sqrt{N}$
- Solution is to sample points "randomly" but also
  - … "equally spaced"
  - … avoiding clustering

Halton's Sequence

- A *quasi*-random sequence that fills space
- To obtain the j^{th} number in series…
  - Consider a prime number b
  - Write j in base b
  - Reverse the digits of j
  - Add a leading decimal
- In n-dimensions, consider n different primes

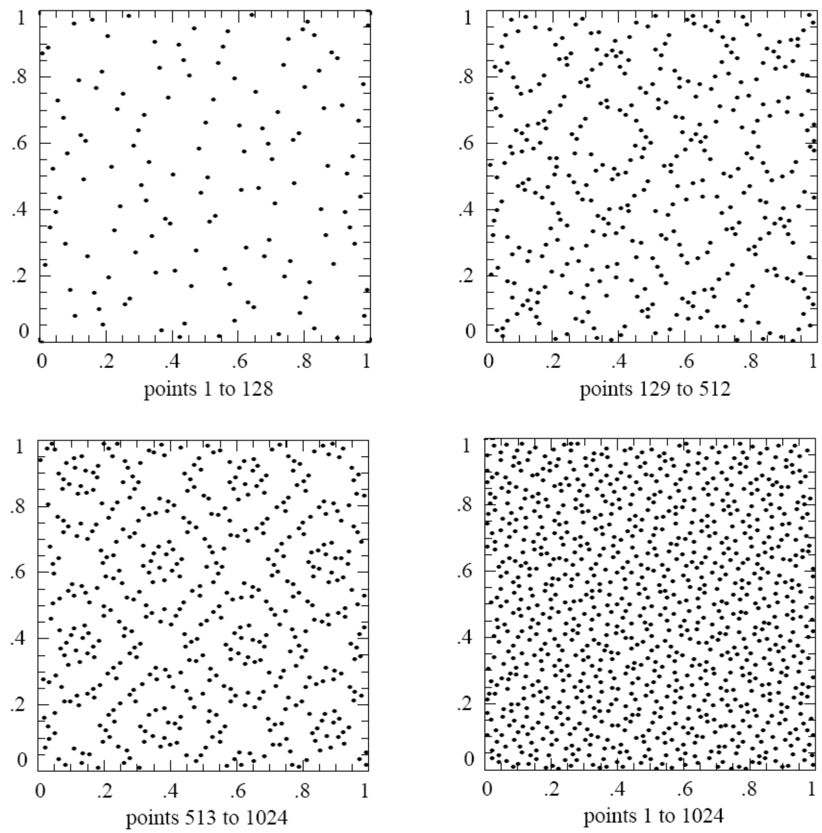
Halton's Sequence (b = 2)

Digits	Reversed	Base 10
0	.0	0.000
1	.1	0.500
10	.01	0.250
11	.11	0.750
100	.001	0.125
101	.101	0.625
110	.011	0.375
111	.111	0.875

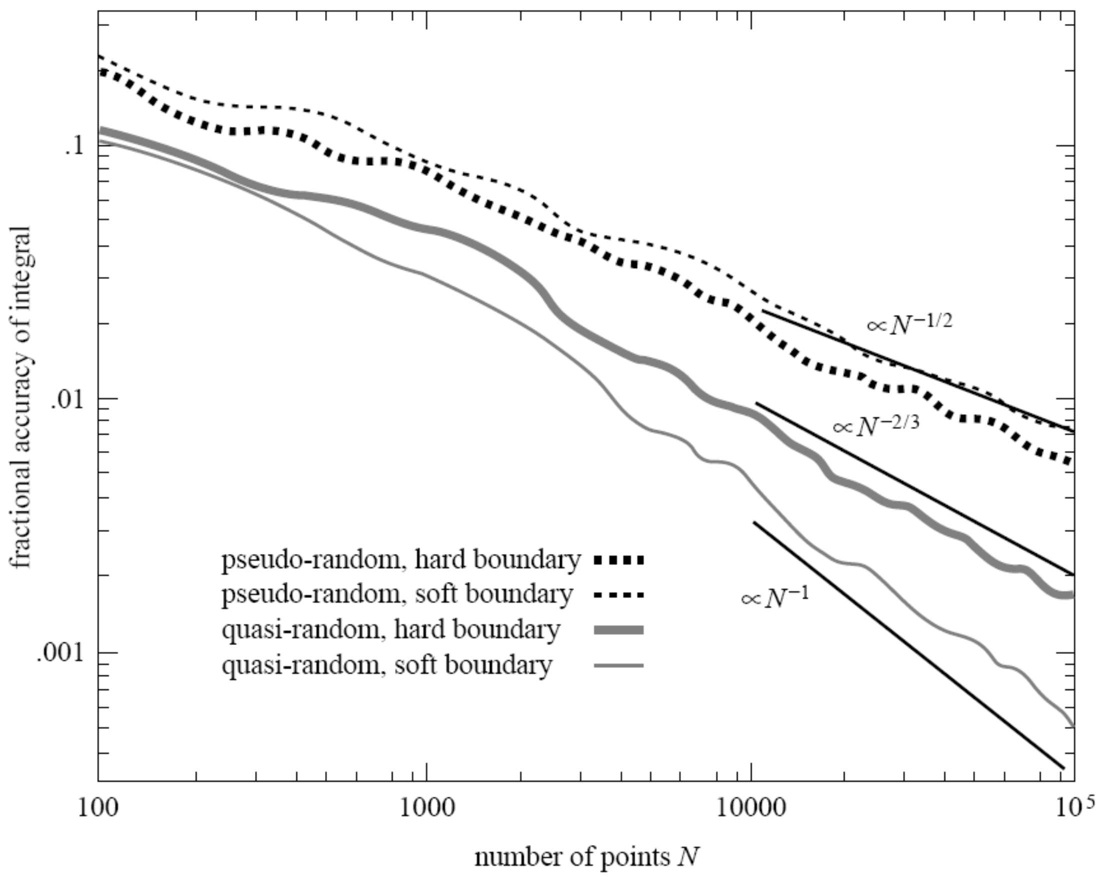
Halton’s Sequence (b = 3)

Digits	Reverse	Base 10
0	.0	0.000
1	.1	0.333
2	.2	0.667
10	.01	0.111
11	.11	0.444
12	.21	0.778
20	.02	0.222
21	.12	0.556
22	.22	0.889

Sobol's Sequence



Advantages of Quasi-Random Sequences



Quasi-Random Sequences

- Although Halton's sequence is intuitive, it is a bit cumbersome to code
- Other sequences (such as Sobol's sequence) are more commonly used in practice
- They can all greatly improve accuracy of Monte-Carlo integrals

So far …

- Random sampling of points is simplest…
- … but quasi-random sampling is better

- Let’s examine why in a bit more detail.

Stratified Sampling, 2 regions

- Use random sampling within each one

- The estimated average of the function is …

$$\langle f \rangle' \equiv \frac{1}{2}\left(\langle f \rangle_a + \langle f \rangle_b\right)$$

- With variance …

$$\mathrm{Var}\left(\langle f \rangle'\right) = \frac{1}{4}\left[\mathrm{Var}\left(\langle f \rangle_a\right) + \mathrm{Var}\left(\langle f \rangle_b\right)\right]$$

Stratified Sampling Improves Accuracy!

- Without stratifying, variance would be:

$$\mathrm{Var}(f) = \frac{1}{2}\left[\mathrm{Var}_a(f) + \mathrm{Var}_b(f)\right] + \frac{1}{4}\left(\langle\langle f\rangle\rangle_a - \langle\langle f\rangle\rangle_b\right)^2$$

- Extra term reflects differences in region specific means
- <<>> operator denotes true average

Stratified Sampling, with Different Numbers of Points

- In this setting, expected variance of stratified estimate is:

$$\mathrm{Var}\left(\langle f \rangle'\right) = \frac{1}{4}\left[\frac{\mathrm{Var}_a\left(f\right)}{N_a} + \frac{\mathrm{Var}_b\left(f\right)}{N - N_a}\right]$$

- Which is minimized when:

$$\frac{N_a}{N} = \frac{\sigma_a}{\sigma_a + \sigma_b}$$

Recursive Stratified Sampling

- Given total number of evaluations N

- Sample a few points at random
- Identify optimal bisection
- Integrate each half separately
  - Repeating the steps above in each half that is not too small…

Practical Nuances

- Instead of examining variance in each half
  - Check minimum and maximum function values
- Weights for allocating points are heuristic
  - Attenuated compared to idealized weights
- Should the splits generate equal halves?

C Code: Constants

```
/* Don't split less than these points */
#define MINPOINTS             60

/* Minimum allocation for each half */
#define MINSPLIT              15

/* Minimum points for exploring split */
#define EXPLORE_MIN           10

/* Maximum points for exploring split */
#define EXPLORE_MAX           100

/* Proportion of points for exploration */
#define EXPLORE_PROPORTION    0.10

/* A very large value */
#define VERY_LARGE            1.0e20
```

C Code: Recursive Integration (I)

```
double RecursiveIntegration(double (* f)(double *, int),
                double * lo, double * hi, int dim, int N)
   {
   int RandD; double save, result, totalvar, var0;
   double * midpoint = alloc_vector(dim);
   double ** min = alloc_matrix(2, dim);
   double ** max = alloc_matrix(2, dim);

   if (N < MINPOINTS) return Integrate(f, lo, hi, dim, N);

   SetupIntegration(lo, hi, midpoint, min, max, dim, N, RandD);
   ExploreIntegral(f, lo, hi, midpoint, min, max, dim, RandD);
   int split = ChooseSplit(min, max, dim, totalvar, var0);

   int points0 = N * var0 / totalvar;
   if (points0 < MINSPLIT) points0 = MINSPLIT;
```

C Code: Recursive Integration (II)

```
save = hi[split]; hi[split] = midpoint[split];
result = RecursiveIntegration(f, lo, hi, dim, points0);
hi[split] = save;

save = lo[split]; lo[split] = midpoint[split];
result += RecursiveIntegration(f, lo, hi, dim, N - points0);
lo[split] = save;

free_vector(midpoint, dim);
free_matrix(min, 2, dim);
free_matrix(max, 2, dim);

return result;
}
```

Helper Functions…

- The main code delegates nearly all its tasks
- SetupIntegration()
  - Initialize variables
  - Decide how many points to invest in R&D
- ExploreIntegral()
  - Sample points and collect information for bisection
- ChooseSplit()
  - Decide how best to divide volume

Helper Function I

```
void SetupIntegration(double * lo, double * hi, double * midpoint,
                      double ** min, double ** max, int dim, int & N, int & RandD)
   {
   // Calculate midpoint for the current region
   for (int j = 0; j < dim; j++)
      {
      midpoint[j] = 0.5 * (lo[j] + hi[j]);
      min[0][j] = min[1][j] =  VERY_LARGE;
      max[0][j] = max[1][j] = -VERY_LARGE;
      }

   // Allocate some points to explore the function...
   RandD = N * EXPLORE_PROPORTION;

   if (RandD < EXPLORE_MIN) RandD = EXPLORE_MIN;
   if (RandD > EXPLORE_MAX) RandD = EXPLORE_MAX;

   N -= RandD;
   }
```

Helper Function II

```
void ExploreIntegral(double (*f)(double *, int),
           double * lo, double * hi, double * midpoint,
           double ** min, double ** max, int dim, int N)
   {
   double * point = alloc_vector(dim);

   for (int n = 0; n < N; n++)
      {
      SamplePoint(point, lo, hi, dim);
      double fx = f(point, dim);

      for (int j = 0; j < dim; j++)
         {
         int half = point[j] > midpoint[j];

         max[half][j] = fx > max[half][j] ? fx : max[half][j];
         min[half][j] = fx < min[half][j] ? fx : min[half][j];
         }
      }
   free_vector(point, dim);
   }
```

Helper Function III

```
int ChooseSplit(double ** min, double ** max, int dim,
                double & var, double & var0)
   {
   int split = -1;

   // Choose the region giving biggest reduction in the variance
   for (int j = 0; j < dim; j++)
      // have we got two points on each half of the region?
      if (max[0][j] > min[0][j] && max[1][j] > min[1][j])
         {
         // The lines below use the empirical weighting
         double sigma0 = pow(max[0][j] - min[0][j], 2.0 / 3.0);
         double sigma1 = pow(max[1][j] - min[1][j], 2.0 / 3.0);

         double sigma = sigma0 + sigma1;

         if (split == -1 || sigma < var)
            { split = j; var = sigma; var0 = sigma0; }
         }

   if (split == -1)
      { var0 = 1.0; var = 2.0; split = Random() * dim; }

   return split;
   }
```

Test Results

- Integrating a bivariate normal distribution

- Simple Monte-Carlo Integration
  - 100, 1000, 10000, 100000 evaluations
  - .002, .0006, .0002, .00006 standard error

- Recursive stratified sampling
  - 100, 1000, 10000, 100000 evaluations
  - .001, .0001, .00001, .000001 standard error

Enhancements

- Randomize splits a little bit …
- Use Halton’s sequence (or similar) to select points

Today

- Monte Carlo Integration
  - Randomly distributed points
  - Points selected to fill space
  - Points targeted to high variance regions
- The last two strategies can be combined!

Recommended Reading

- Numerical Recipes
  - Chapter 7.6 – 7.8
- Available online at:
  - http://www.nr.com