Math 4/896: Seminar in Mathematics Topic: Inverse Theory

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AvH 10

Quality of Least Squares

A very nontrivial result which we assume:

Theorem

Let G have full column rank and m the least squares solution for the scaled inverse problem. The statistic

$$\|\mathbf{d}_{W} - G_{W}\mathbf{m}\|_{2}^{2} = \sum_{i=1}^{m} (d_{i} - (Gm_{L_{2}})_{i})^{2} / \sigma_{i}^{2}$$

in the random variable **d** has a chi-square distribution with $\nu = m - n$ degrees of freedom.

This provided us with a statistical assessment (the chi-square test) of the quality of our data. We need the idea of the p-value of the test, the probability of obtaining a larger chi-square value than the one actually obtained:

$$p=\int_{\chi_{obs}^{2}}^{\infty}f_{\chi^{2}}\left(x\right) dx.$$

Interpretation of p

As a random variable, the p-value is uniformly distributed between zero and one. This can be very informative:

- "Normal sized" p: we probably have an acceptable fit
- ② Extremely small p: data is very unlikely, so model $G\mathbf{m} = \mathbf{d}$ may be wrong or data may have larger errors than estimated
- Extremely large p (i.e., very close to 1): fit to model is almost exact, which may be too good to be true.

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Uniform Distributions

Reason for uniform distribution:

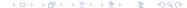
Theorem

Let X have a continuous c.d.f. F(x) such that F(x) is strictly increasing where 0 < x < 1. Then the r.v. Y = F(X) is uniformly distributed on the interval (0,1)

Proof sketch:

- Calculate $P(Y \le y)$ using fact that F has an inverse function F^{-1} .
- Use the fact that $P(X \le x) = F(x)$ to prove that $P(Y \le y) = y$.

Application: One can use this to generate random samples for X.



An Example

Let's resume our experiment from above. Open the script Lecture8.m and have a look. Then run Matlab on it and resume calculations.

> % now set up for calculating the p-value of the test under both scenarios.

```
>chiobs1 = norm(data - G*mapprox1)^2
>chiobs2 = norm(W*(data - G*mapprox2))^2
>help chis_pdf
>p1 = 1 - chis_cdf(chiobs1,m-n)
>p2 = 1 - chis_cdf(chiobs2,m-n)
% How do we interpret these results?
% Now put the bad estimate to the real test
How do we interpret these results?
```

More Conceptual Tools

Examine and use the MVN theorems of ProbStatLectures to compute the expectation and variance of the r.v. \mathbf{m} , where \mathbf{m} is the modified least squares solution, G has full column rank and \mathbf{d} is a vector of independent r.v.'s.

 Each entry of m is a linear combination of independent normally distributed variables, since

$$\mathbf{m} = \left(G_W^T G_W \right)^{-1} G_W^T \mathbf{d}_W.$$

- The weighted data $\mathbf{d}_W = W\mathbf{d}$ has covariance matrix I.
- Deduce that $Cov(\mathbf{m}) = (G_W^T G_W)^{-1}$.
- Note simplification if variances are constant: $Cov(\mathbf{m}) = \sigma^2 (G^T G)^{-1}$.



Next examine the mean of m and deduce from the facts that

$$E\left[\mathbf{d}_{W}\right] = W\mathbf{d}_{true} \text{ and } G_{W}\mathbf{m}_{true} = \mathbf{d}_{true}$$

and MVN facts that

- \bullet $E[m] = m_{true}$
- Hence, modified least squares solution is an unbiased estimator of m_{true}.
- Hence we can construct a confidence interval for our experiment:

$$\mathbf{m} \pm 1.96 \cdot \text{diag} \left(\text{Cov} \left(\mathbf{m} \right) \right)^{1/2}$$

 What if the (constant) variance is unknown? Student's t to the rescue!



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Outliers

These are discordant data, possibly due to other error or simply bad luck. What to do?

- Use statistical estimation to discard the outliers.
- Use a different norm from $\|\cdot\|_2$. The 1-norm is an alternative, but this makes matters much more complicated! Consider the optimization problem

$$\left\|\mathbf{d} - G\mathbf{m}_{L_2}\right\|_1 = \min_{\mathbf{m}} \left\|\mathbf{d} - G\mathbf{m}\right\|_1$$

A Motivating Example: Integral Equations

Contanimant Transport

Let C(x,t) be the concentration of a pollutant at point x in a linear stream, time t, where $0 \le x < \infty$ and $0 \le t \le T$. The defining model

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x}$$

$$C(0,t) = C_{in}(t)$$

$$C(x,t) \to 0, x \to \infty$$

$$C(x,0) = C_0(x)$$

Solution:

$$C(x,T) = \int_0^T C_{in}(t) f(x,T-t) dt,$$

where

$$f(x,\tau) = \frac{x}{2\sqrt{\pi D\tau^3}} e^{-(x-v\tau)^2/(4D\tau)}$$

The Inverse Problem

Problem:

Given simultaneous measurements at time \mathcal{T} , to estimate the contaminant inflow history.

More generally

Problem:

Given the IFK

$$d(s) = \int_a^b g(x, s) m(x) dx$$

and a finite sample of values $d(s_i)$, to estimate parameter m(x).

- Quadrature
- 2 Representers
- Orthogonal representers

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