Nonparametric Inference and the Dark Energy Equation of State

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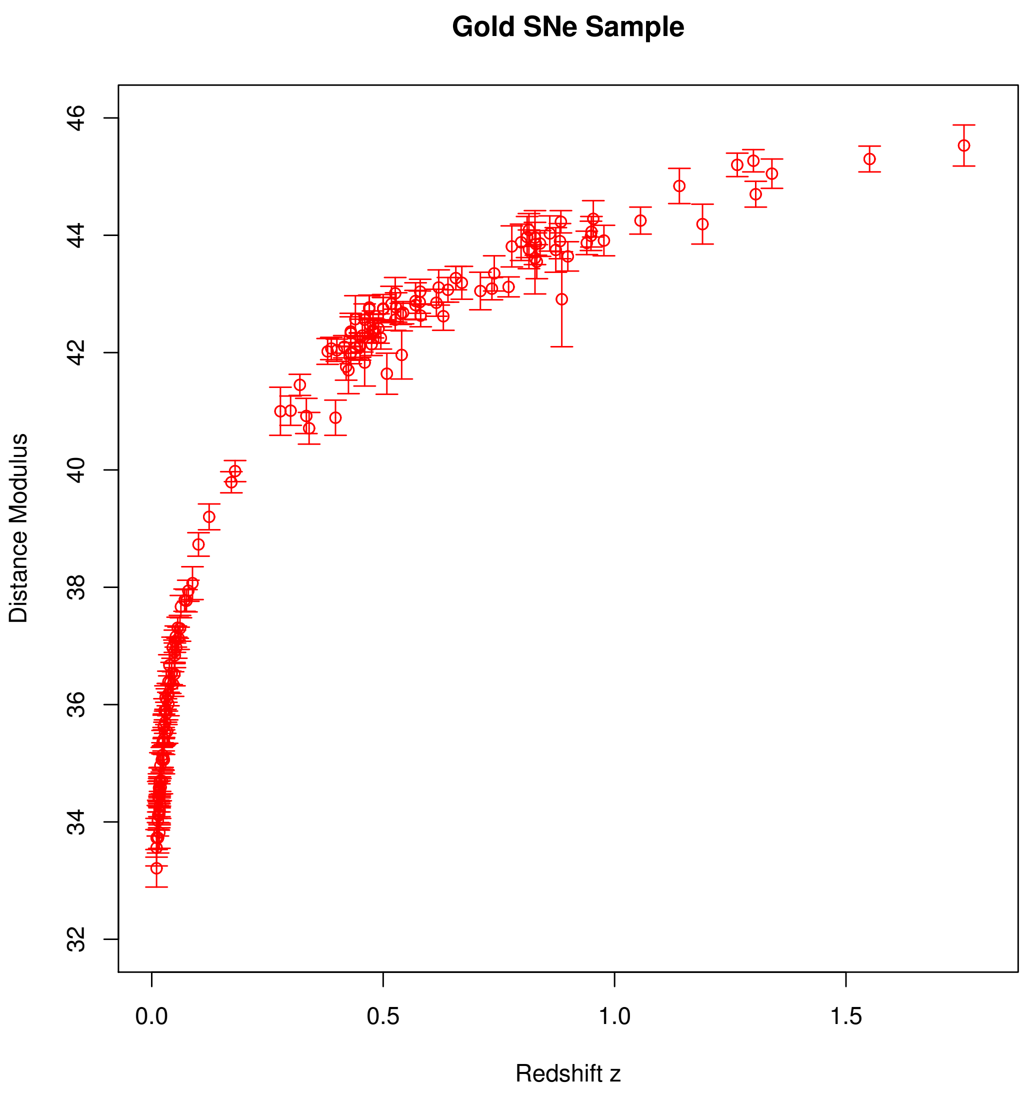
A Small-Sample Story for a Large-Sample World

- The flood of data in astronomy is only just beginning.
- Such data open up new questions and raise new challenges.
- Nonparametric methods are well suited to these new problems.
  - Cosmic Microwave Background (Genovese et al. 2004, Bryan et al. 2005)
  - Galaxy Evolution (e.g., Rojas et al. 2006)
  - Galaxy Spectra (work in progress)
  - Dark Energy (e.g., Daly and Djorgovski 2004, 2005; and below)
- So, in this terabyte age, I want to illustrate this potential with a data set of mere hundreds.



Gold SNe Sample
Distance Modulus
Redshift z
32
34
36
38
40
42
44
46
0.0
0.5
1.0
1.5

Road Map

1. Dark Energy
2. Nonparametric Inference
3. Derivative Estimation as an Inverse Problem
4. Inference for the Dark Energy Equation of State

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Preliminaries

- The Expanding Universe

  Scale factor $a(t)$ indicates relative expansion of the universe.
  ($a(t_0) = 1$ where t_0 is current age of universe.)

  Redshift z is an observable shift in the wavelength of light from a distant object that is induced by the expansion of the universe.

$$1 + z = \frac{\lambda_{\mathrm{obs}}}{\lambda_{\mathrm{emit}}} = \frac{a(t_{\mathrm{obs}})}{a(t_{\mathrm{emit}})}.$$

  Hubble parameter $H(t) = \frac{\dot{a}(t)}{a(t)}$. ($H_0 = H(t_0)$ is the Hubble "constant".)

- The Distance-Redshift Relation

  The relationship between objects' distances and redshifts contains fundamental information about the Universe's geometry.

  Hubble's Law, $z = H_0 d$, is reasonably accurate for small distances d.

Dark Energy

- Accelerating Expansion (Reiss et al. 2004, Perlmutter et al. 2004)

  Type Ia supernovae can serve as a "standard candle".

  Observations of many supernovae reveal that the expansion of the universe is *accelerating*.

  This conclusion is supported by other, independent, measurements, including the Cosmic Microwave Background (Spergel et al. 2003) and large-scale structure (Verde et al. 2002).

- Einstein's "mistake," Cosmological Constant, and Vacuum Energy
- This raises several puzzles. What's going on?
  - Mistaken assumptions, models, or data analysis
  - A failure of General Relativity
  - Anthropic Selection
  - Dark Energy

Dark Energy (cont'd)

- Dark Energy is a smoothly-distributed energy density that dominates the universe ($\sim$ 74% versus $\sim$ 4% for baryonic matter) and provides a negative pressure acting in opposition to gravity.
- What does the acceleration imply about dark energy?

  Let $\rho = \rho_{\rm matter} + \rho_{\rm radiation} + \rho_{\rm DE} + \cdots$ be the total energy density in the universe.

  Friedmann equation:

$$H^2(t) = \left(\frac{\dot{a}(t)}{a(t)}\right)^2 = \frac{8\pi G}{3}\rho - \frac{\kappa}{a^2(t)}$$

  or equivalently,

$$\dot{a}^2 = \frac{8\pi G}{3}a^2\rho - \kappa.$$

  Acceleration implies that $a^2\rho$ must increase.

  Neither matter ($\rho_{\rm matter} \propto a^{-3}$) nor radiation ($\rho_{\rm radiation} \propto a^{-4}$) can do this.
  A cosmological constant ($\rho_{\rm DE} \propto a^0$) could.

Dark Energy (cont'd)

- How do we quantify dark energy?

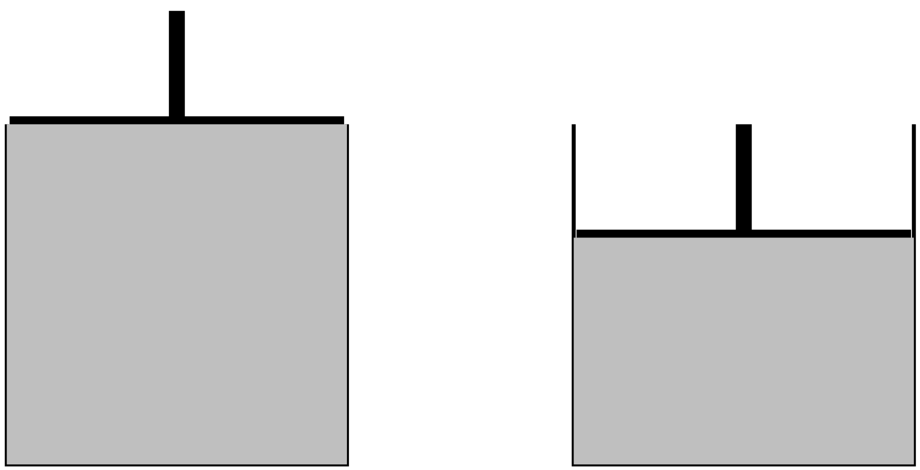
  We can attempt to make inferences about ρ directly.

  Alternatively, we can look at the equation of state (cf. ideal gas law).

  Let p_{DE} and ρ_{DE} be the pressure and energy density of dark energy, then the equation of state w relates these by

$$p_{\mathrm{DE}} = w\rho_{\mathrm{DE}}.$$

  For a cosmological constant, $w = -1$.



$$\text{Work} = -p_{\mathrm{DE}}\Delta V$$
$$\Delta\text{Energy} = \rho_{\mathrm{DE}}\Delta V$$
$$\implies p_{\mathrm{DE}} = -\rho_{\mathrm{DE}}$$

Dark Energy (cont'd)

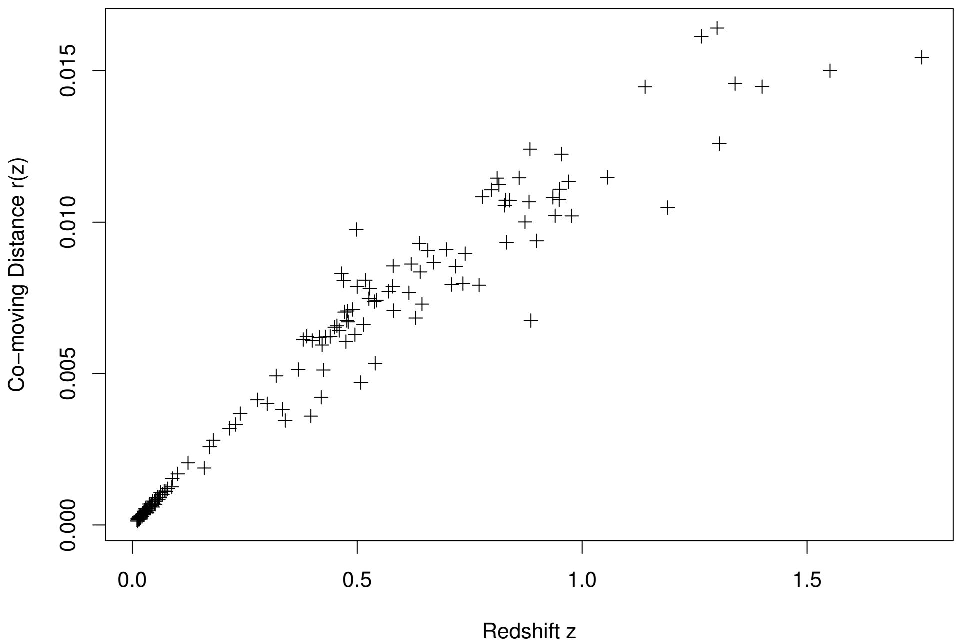
- The supernova data give us a way to infer the equation of state

  Roughly, we get

$$Y_i = r(z_i) + \sigma_i \epsilon_i, \qquad i = 1, \ldots, n,$$

where r is a measure of distance at each redshift z_i. Then,

$$w(z) = \frac{H_0^2 \Omega_M (1+z)^3 + \frac{2}{3} \frac{r''(z)}{(r'(z))^3}}{H_0^2 \Omega_M (1+z)^3 - \frac{1}{(r'(z))^2}} \equiv T(r', r'').$$



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Nonparametric Inference

Goal: make sharp inferences about unknown functions with a minimum of assumptions.

Constructing good estimators is important, but an accurate assessment of uncertainty is critical.

Why use nonparametric methods?

1. When we don't have a well-justified parametric (finite-dimensional) model for the object of interest.
2. When we have a well-justified parametric model but have enough data to go after even more detail.
3. When we can do as well (or better) more simply.
4. As a way of assessing sensitivity to model assumptions.

Aside: What's in a name?

The term "nonparametric" is unfortunate, although now firmly established.

- There is a parameter in these models – the unknown function.
- Loosely speaking, the contrast between nonparametric and parametric is an infinite-dimensinoal parameter versus a finite-dimensional parameter.
- We have only n data. But with a nonparametric analysis, the dimension of the fit grows with n; in a parametric analysis, it is fixed for all n.
- These methods go beyond the rank-based testing of classical nonparametric statistics.

The Nonparametric Regression Problem

Observe data (X_i, Y_i) for $i = 1, \ldots, n$ where

$$Y_i = f(X_i) + \epsilon_i,$$

where $\mathsf{E}(\epsilon_i) = 0$ and the X_is can be fixed (x_i) or random.

Leading cases: 1. $x_i = i/n$ and $\mathsf{Cov}(\boldsymbol{\epsilon}) \equiv \Sigma = \sigma^2 I$.

2. X_i IID g and $\mathsf{Cov}(\boldsymbol{\epsilon}) \equiv \Sigma = \sigma^2 I$.

Key Assumption: $f \in \mathcal{F}$ for some infinite dimensional space $\mathcal{F}$.

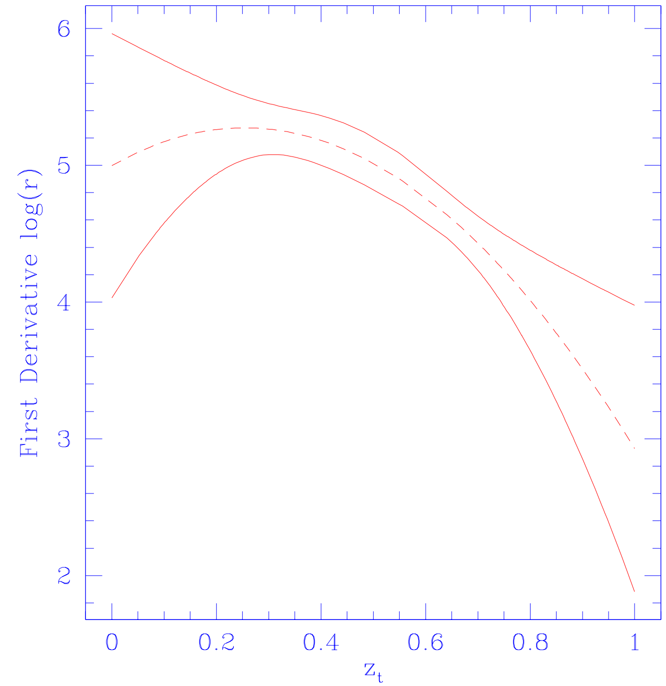
Examples

1. Sobolev: $\mathcal{F} \equiv \mathcal{W}_p(C) = \left\{ f \colon \int |f|^2 < \infty \text{ and } \int |f^{(p)}|^2 \le C^2 \right\}$
2. Lipschitz: $\mathcal{F} \equiv \mathcal{H}(A) = \{ f \colon |f(x) - f(y)| \le A|x - y|, \text{ for all } x, y \}$

Goal: Make inferences about f or about specific features of f.

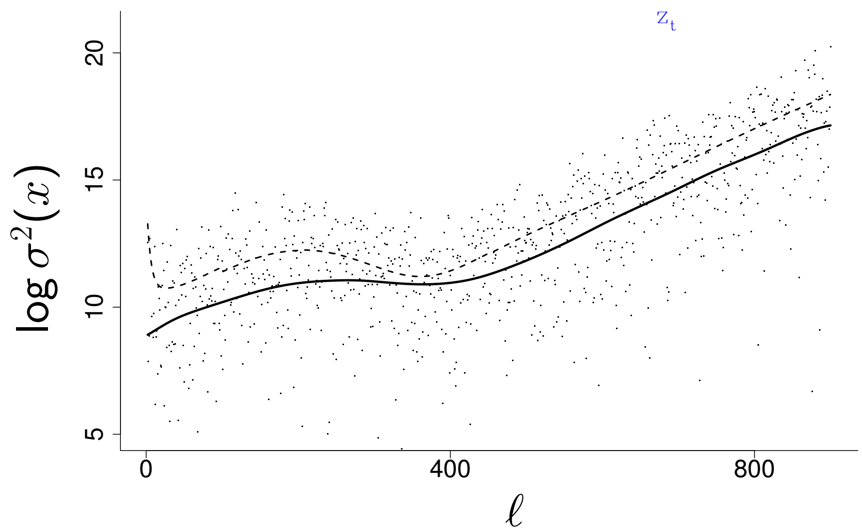
Variants of the Problem

- Inference for Derivatives of f
- Estimating Variance functions
- Regression in High dimensions
- Inferences about specific functionals of f



Related Problems:

- Density Estimation
- Spectral Density Estimation



Rate-Optimal Estimators

Choose a performance measure, or risk function, e.g.,
$R(\widehat{f}, f) = \mathsf{E} \int (\widehat{f} - f)^2$ or $R(\widehat{f}, f) = \mathsf{E}|\widehat{f}(x_0) - f(x_0)|^2)$

Want $\widehat{f}$ that minimizes worst-case risk over $\mathcal{F}$ (minimax).

But typically must settle for achieving the optimal minimax rate of convergence r_n:

$$\inf_{\widehat{f}_n} \sup_{f \in \mathcal{F}} R(\widehat{f}_n, f) \asymp r_n$$

In infinite-dimensional problems, $r_n \sqrt{n} \to \infty$.

For example, $r_n = n^{-\frac{2p}{2p+1}}$ on $\mathcal{W}_p$.

Rate-optimal estimators exist for a wide variety of spaces and risk functions.

Adaptive Estimators

It's unsatisfying to depend too strongly on intangible assumptions such as whether $f \in \mathcal{W}_p(C)$ or $f \in \mathcal{H}(A)$.

Instead, we want procedures to *adapt* to the unknown smoothness.

For example, $\widehat{f}_n$ is a *(rate) adaptive procedure* over the $\mathcal{W}_p$ spaces if when $f \in \mathcal{W}_p$

$$\widehat{f}_n \to f \text{ at rate } n^{-2p/2p+1}$$

without knowing p.

Rate adaptive estimators exist over a variety of function families and over a range of norms (or semi-norms).

Adaptive confidence sets?? Limited at best.

Inference Not So Easy

Using a rate-optimal smoothing parameter gives

$$\text{bias}^2 \approx \text{var}.$$

Loosely, if $\widetilde{f} = \mathsf{E}\widehat{f}$ and $s = \sqrt{\text{Var}\,\widehat{f}}$, then

$$\frac{\widehat{f} - f}{s} = \frac{\widehat{f} - \widetilde{f}}{s} + \frac{\widetilde{f} - f}{s} \approx \mathsf{N}(0,1) + \frac{\text{bias}}{\sqrt{\text{var}}}.$$

So, "$\widehat{f} \pm 2s$" undercovers.

Two common solutions in the literature:

– Bias Correction: Shift confidence set by estimated bias.

– Undersmoothing: Smooth so that var dominates bias^2.

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Derivative Estimation as an Inverse Problem

We can think of derivative estimation as an ill-posed inverse problem.

Suppose we have data

$$Y_i = r(z_i) + \sigma_i \epsilon_i$$

and want to make inferences about $f \equiv r'$. Then we can write (in vector form)

$$Y = Kf + \Sigma^{1/2}\epsilon$$

where the operator $K = (K_1, \ldots, K_n)$ maps functions to $\mathbb{R}^n$ and where $K_i = \int_0^{z_i}$.

Create an orthonormal basis $\phi_1, \ldots, \phi_n$ from the eigenfunctions of K^*K with associated eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$.

Here, K^* is the adjoint of K given by

$$K^* u = \sum_{i=1}^{n} u_i 1_{[0,z_i]}.$$

Derivative Estimation (cont'd)

Then,

$$f = \sum_{j=1}^{n} \beta_j \phi_j + f_\perp$$

$$= \sum_{j=1}^{n} \lambda_j^{-1/2} \langle u_j, Kf \rangle \phi_j + f_\perp,$$

where $u_j = K\phi_j / \|K\phi_j\|$. The $f_\perp$ component is not estimable.

Using an optimal shrinkage scheme,

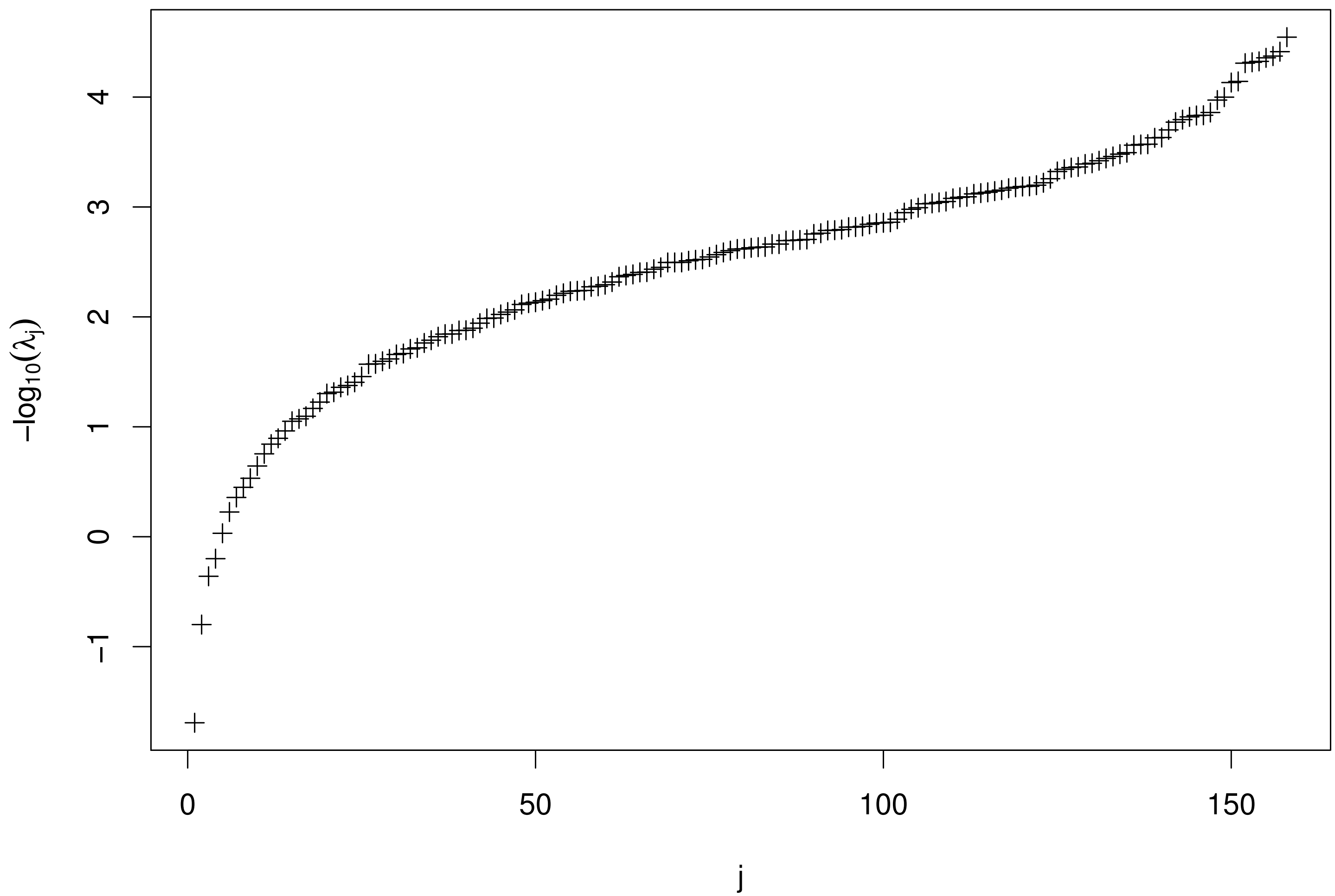
$$MSE \approx \sum_{j=1}^{n} \min(\beta_j^2, \lambda_j^{-1} \tau_j^2),$$

where $\tau_j^2 = \sum_k u_{jk}^2 \sigma_k^2$.

Large components at high order are bad news!

Derivative Estimation (cont'd)

Associated Eigenvalues (as $-\log_{10}\lambda_j$) for the Supernova Data



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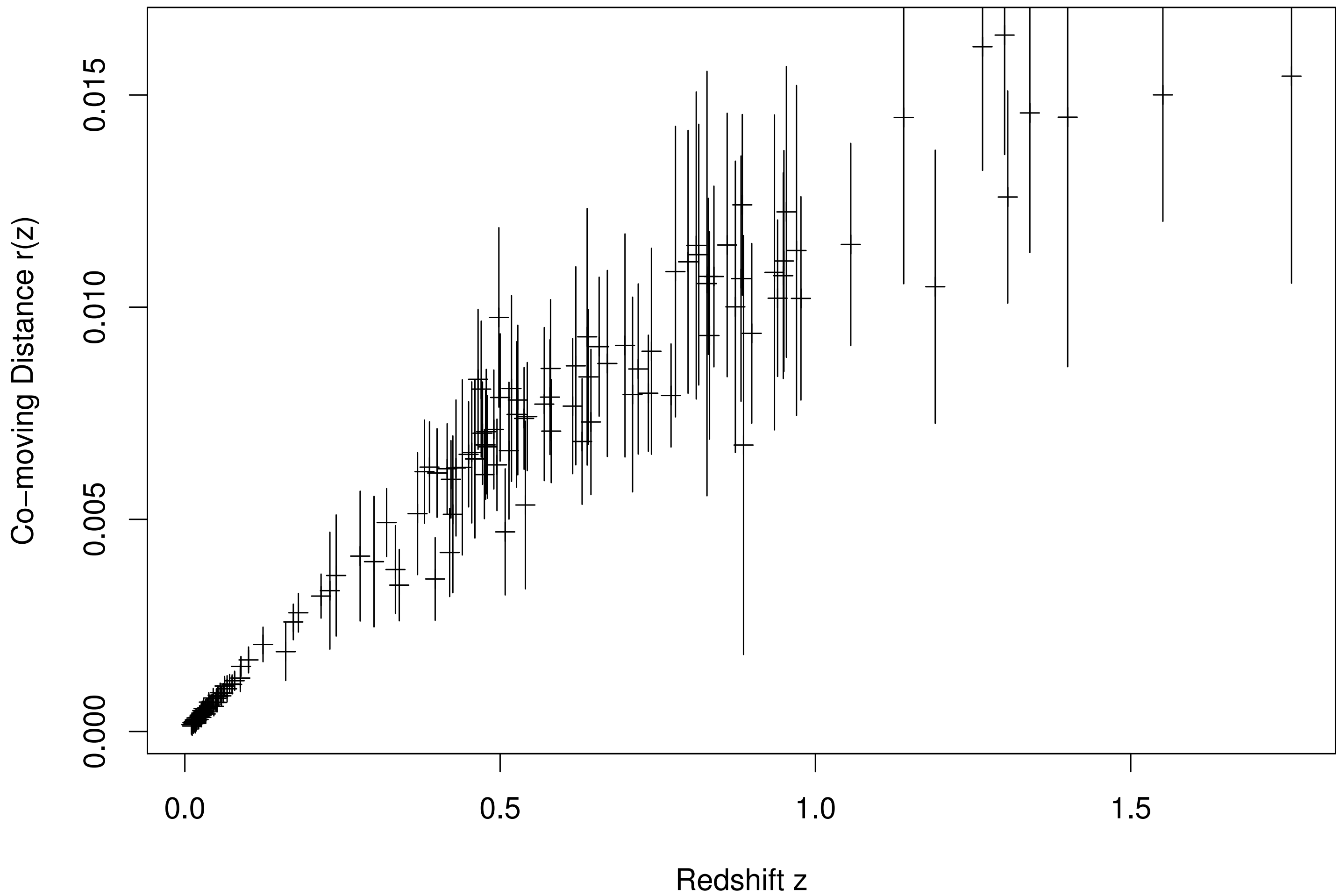
Inference for the Equation of State



Two approaches: Direct testing and nonparametric methods.

Inference (cont'd): Direct Testing

- Let $Q(z)$ be a fixed function, such as $Q(z) \equiv -1$.

  Then, the null hypothesis $H_0 : w = Q$ corresponds to the set of r' solving a differential equation:

  $$\frac{2}{3}(1+z)r''(z)+r'(z)(1+Q(z))-(r'(z))^3 Q(z)H_0^2\Omega_m(1+z)^3 = 0.$$

  This can be solved.

- The result is a family of solutions parameterized by $r'(0)$.

- Invert goodness of fit tests to generate a confidence set of those solutions in the family that are consistent with the data.

  Account for the uncertainty in $H_0^2\Omega_m$.

- Easily generalizes to any finite-dimensional family of $Q(z)$s.

Inference (cont'd): Nonparametric Methods

- Orthonormal basis expansion (singular functions or wavelet-vaguelete) or local polynomial regression
- Double reflection drastically reduces boundary bias in this problem.
- Minimize an unbiased estimate of risk $\widehat{R}$ to select tuning parameters
- Confidence bands via tube formula (Sun and Loader 1994).

  $$\widehat{f} \pm c\,\mathrm{se}(\widehat{f})$$

  where, c solves

  $$\alpha = 2(1 - \Phi(c)) + \kappa\phi(c),$$

  where Φ and ϕ are standard Gaussian cdf and density, respectively, and κ is a constant that depends on the procedure but not on f.
- Must account for bias. Commonly used methods of bias adjustment/estimation fail in simulations.

  Use a global estimate of bias to dilate the bands.

Inference (cont'd): Nonparametric Methods

Issue: What should the target of inference be?

- We can target the effective density $\rho_{\mathrm{DE}}/\rho_{\mathrm{crit}}$ or the equation of state w.
- The effective density can be estimated more precisely, but inference is harder: comparing growth rates of various components.
- The equation of state is harder to estimate (nonlinear functional of two derivatives), but inference is relatively straightforward ($w > -1$?).
- This is an empirical question that depends on accurate assessment of uncertainties: that is, good confidence sets.

Results

- Direct Testing: marginal rejection of $H_0 : w = -1$ with $p \approx 0.006$.

  But a 12% increase in standard errors eliminates the effect.

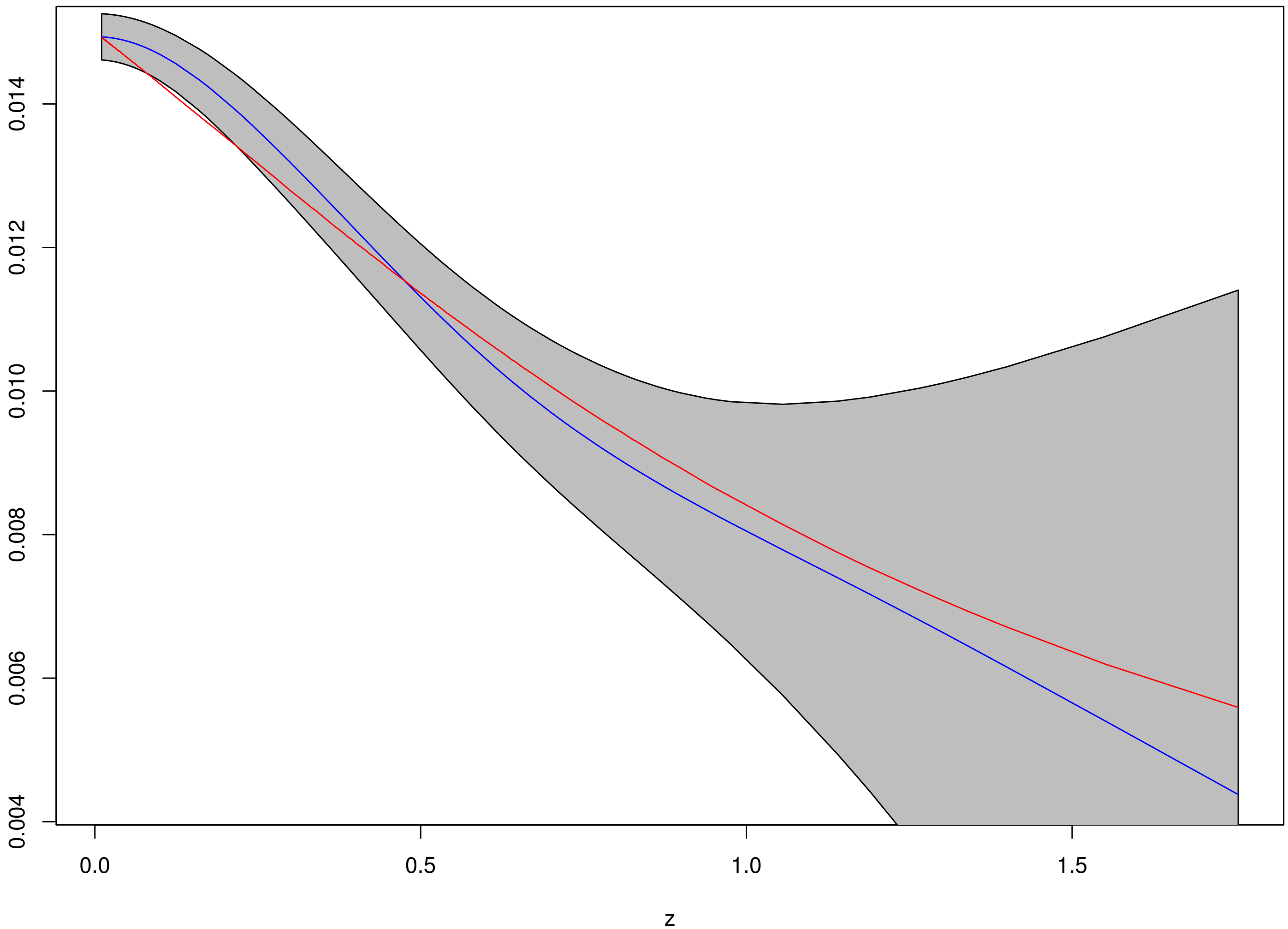
- Nonparametric methods: All the methods generally agree and give results consistent with what we would expect.

  Precision of the estimates is low at high redshift.

  Best fitting r' for $w = -1$ just outside of the confidence bands over small range.

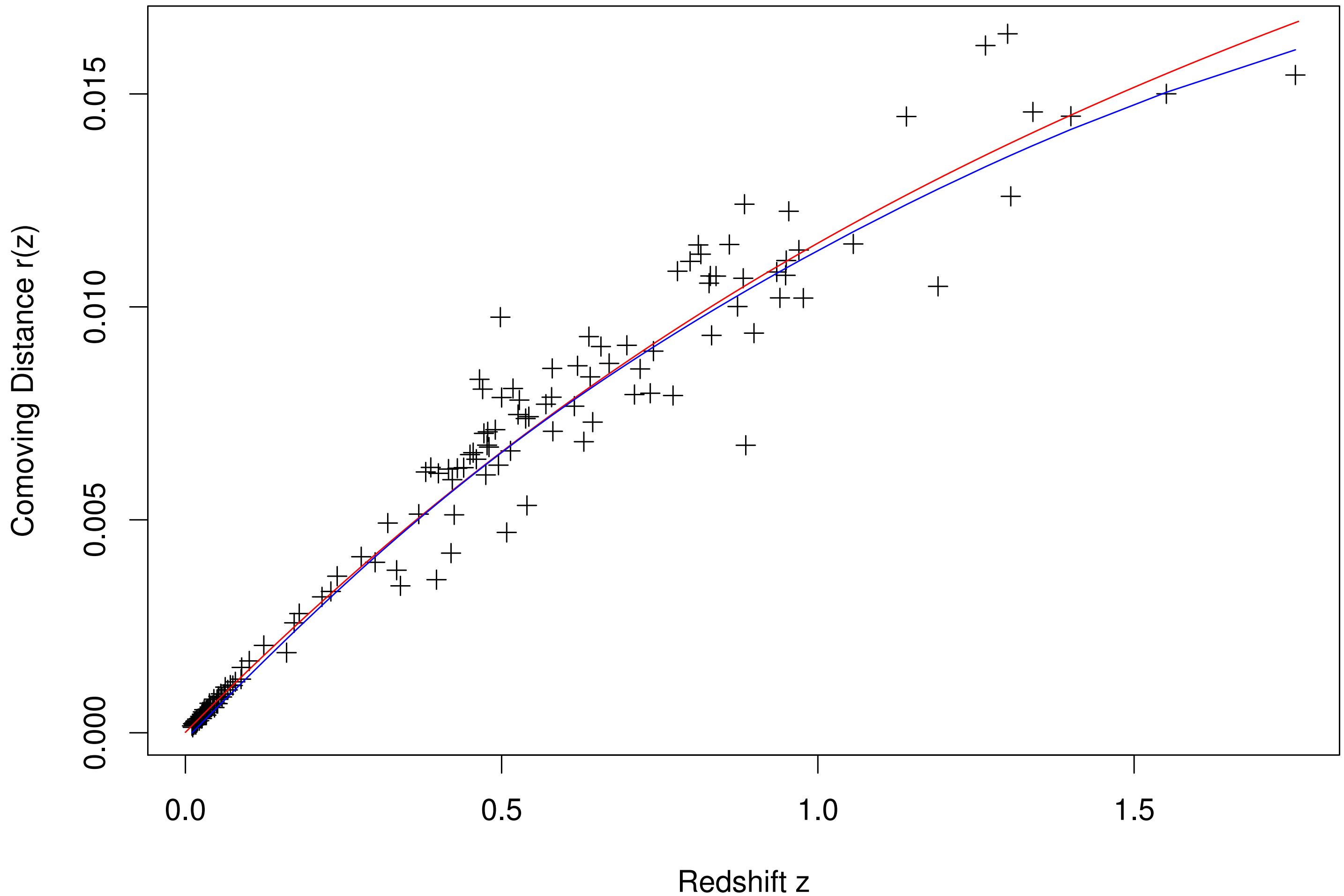
Results (cont'd)

$\widehat{r}'$ with confidence bands ($\widehat{r}'$ within band; $\widehat{r}_0'$ exits band)



Results (cont'd)

$\hat{r}$ from nonparametric and best fitting $\hat{r}_0$ from $w = -1$ solution.



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Take-Home Points

- Nonparametric methods can contribute to fundamental problems in cosmology and astrophysics.

- With the large data sets coming through the pipeline, we can eschew simpler parameterizations and go after the basic physics directly.

- The critical statistical problems focus on constructing inferences for the unknown function (e.g., confidence sets) and for complicated functionals.

Results (cont'd)

$\widehat{\rho}_{\mathrm{DE}}/\rho_{\mathrm{crit}}$ from nonparametric and best fitting from $w = -1$ solution.