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# **NONPARAMETRIC REGRESSION AND MEASUREMENT ERROR**

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**AND CHECK OUT:**

<http://stat.tamu.edu/~carroll> (**most papers available, as well as some matlab software**)

<http://stat.tamu.edu/B3NC> (**Training program in Biology & Bioinformatics**)

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# OUTLINE

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- Model
- Consistent estimation and rates of convergence
- Functional Method: SIMEX
- Structural methods
- Example
- Comments

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## THE BASIC MODEL

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- Nonparametric regression:

$$Y = m(X) + \epsilon, \epsilon \sim (0, \sigma^2)$$

$m(\cdot)$  unspecified

- Measurement error: observe

$$W = X + U, U = \text{Normal}(0, \sigma_u^2) \quad (1)$$

- Assume  $\sigma_u^2$  known for today
- Model (1) is more general than it looks
- Since  $m(\cdot)$  is unspecified, you need only need that (1) holds **after a transformation**

$$\begin{aligned} m(x) &= m[\exp\{\log(x)\}] \\ &= m_*\{\log(x)\}. \end{aligned}$$

- See work by **Nusser, et al.** and **Eckert & Carroll** for such transformations

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## THE BASIC MODEL

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$$Y = m(X) + \epsilon, \epsilon \sim (0, \sigma^2)$$

$$W = X + U, U = \text{Normal}(0, \sigma_u^2)$$

- The issue broadly breaks down into what you must assume about the  $X$ 's
- **Functional**: assume nothing about the  $X$ 's
- **Structural**: assume a (possibly flexible) parametric distribution for the  $X$ 's

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## DECONVOLUTION

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$$Y = m(X) + \epsilon, \epsilon \sim (0, \sigma^2)$$

$$W = X + U, U = \text{Normal}(0, \sigma_u^2)$$

- Estimation of the regression function  $m(\cdot)$  **without knowing the density of  $X$** 
  - Closely related to density deconvolution: estimate density of  $X$  from the  $W$ 's alone
- Density deconvolution (with Stefanski & Hall, 1988) and nonparametric regression (Fan & Truong, 1993) are **nearly impossible**
- No globally consistent estimator of  $m(x)$  can have a rate of convergence faster than  $\log(n)$ 
  - $\log(10,000,000) \approx 16$
  - A sample of size **16** in parametric regression has approximately the same information as a sample of size **10,000,000** for consistent nonparametric regression

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## DECONVOLUTION

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- The deconvolution results mean that if you insist on being consistent nonparametrically
  - and if you insist on no assumptions about the density of the latent  $X$
  - **The you cannot get a decent estimator**
- Fan & Truong constructed an "estimator" using our deconvoluting kernel
  - **It's awful**
  - Bandwidth selection essentially impossible
  - Even cheating and selecting the bandwidth that minimizes MSE, the method has **MSE's an order of magnitude larger** than our other methods
  - Theory really means something here

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## WHAT CAN WE DO??

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$$Y = m(X) + \epsilon$$

$$W = X + U$$

- One method is to allow a **little bit** of inconsistency
  - Still make no assumptions about the density of  $X$
  - But construct an estimator which has less bias than the naive estimator that ignores error
- The naive estimator has a bias of order  $O_p(\sigma_u^2)$
- The **SIMEX estimator** of Cook and Stefanski has a bias of order  $O_p(\sigma_u^6)$
- SIMEX is **general purpose**: kernels, splines, etc.

### Illustration of SIMEX

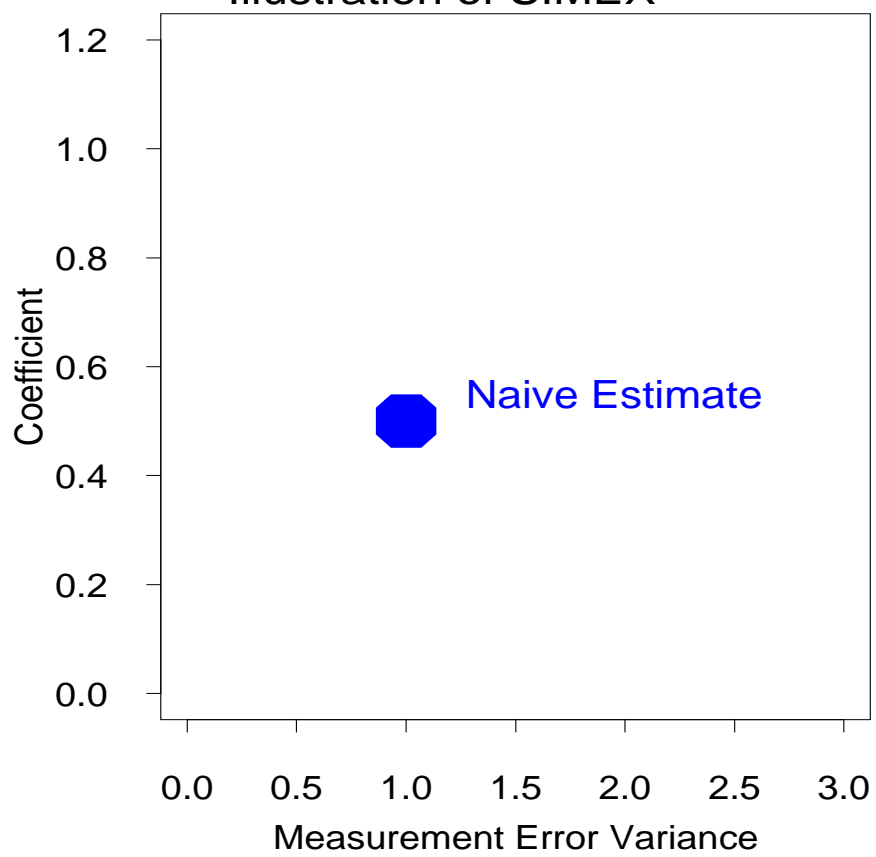


Illustration of SIMEX

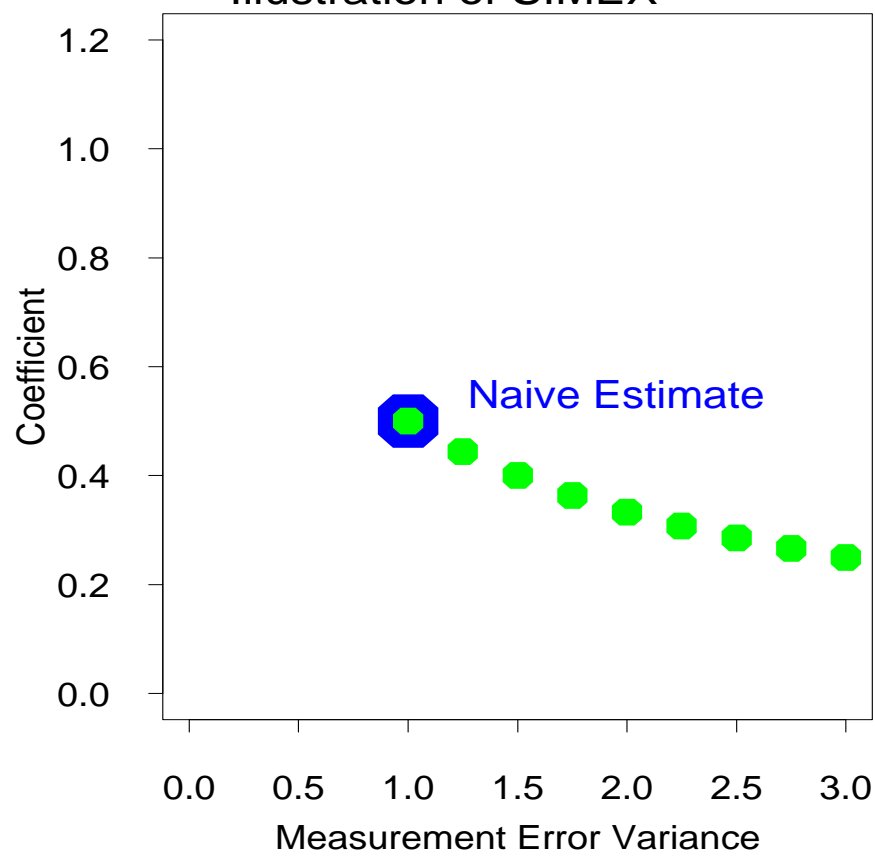


Illustration of SIMEX

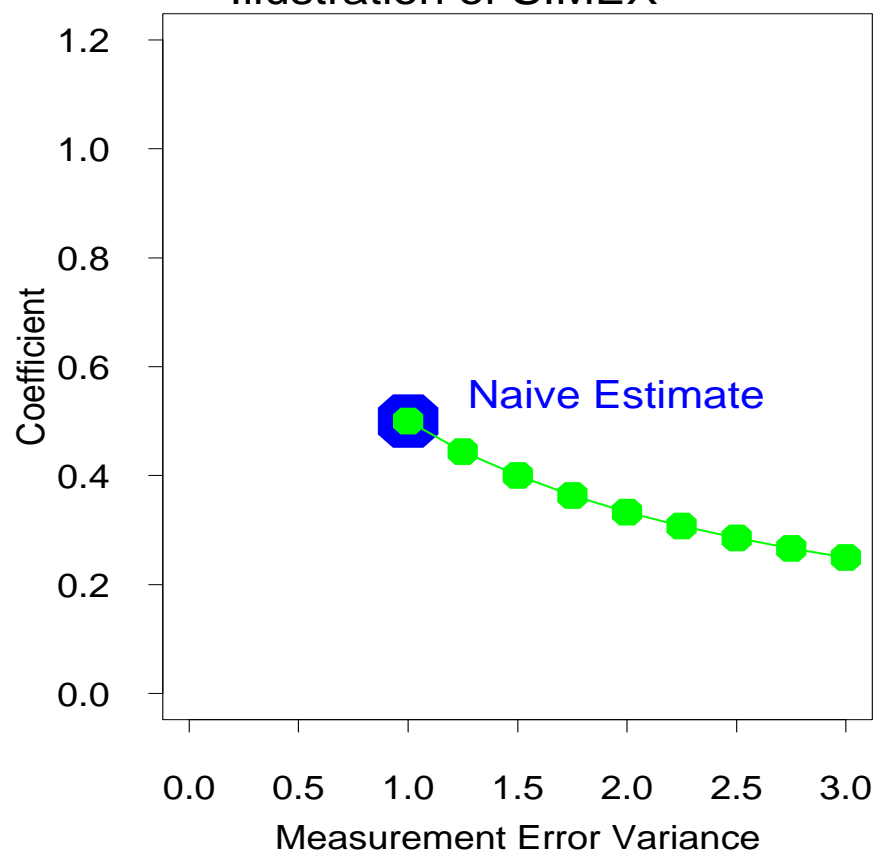
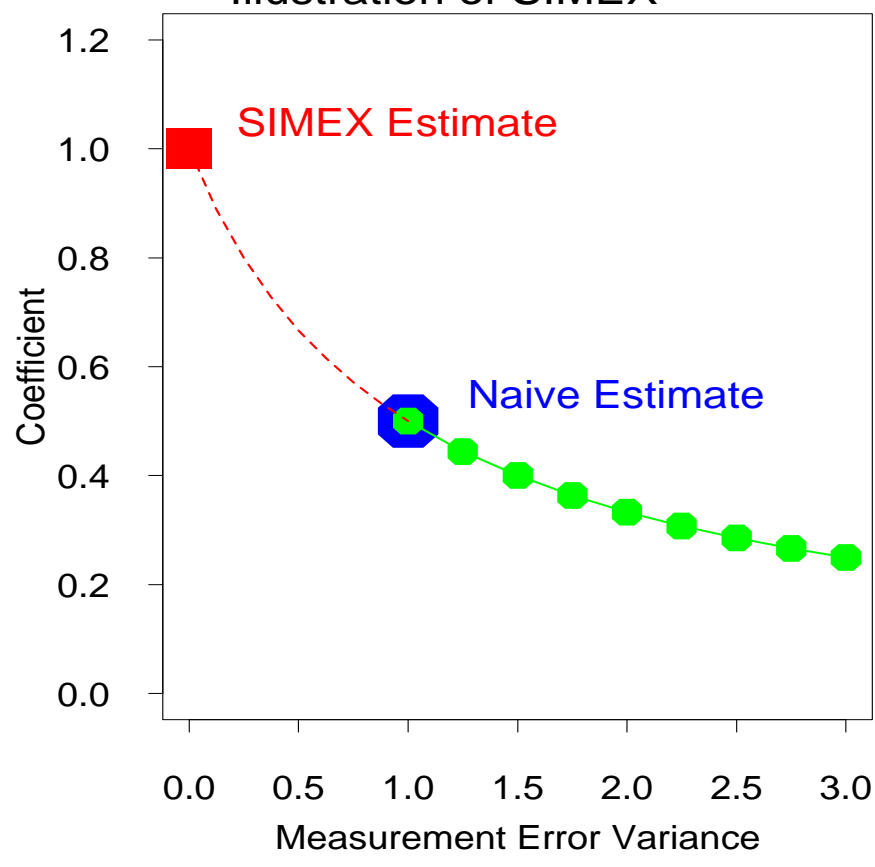


Illustration of SIMEX



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## SIMEX

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- We have derived the asymptotics for SIMEX in kernel regression
  - Bias is  $O_p(\sigma_u^6)$
  - Rate of convergence is standard  $n^{-2/5}$
  - **Approximately consistent** estimation with standard rates
  - Deconvolution is **globally consistent** with slow rates
  - SIMEX has vastly beaten deconvolution in all our simulations
  - Asymptotic variance is the same as if measurement error was ignored, but multiplied by a factor depending only on the extrapolant function
  - linear–quadratic–cubic ratios are 1–9–52

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## SPLINES

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$$Y = m(X) + \epsilon, W = X + U$$

- Write  $m(\cdot)$  in terms of **basis functions**:

$$m(x) = \sum_{j=1}^M \theta_j B_j(x)$$

- **Smoothing splines**
- **P-splines** (Eiler & Marx, with Ruppert, like Splus),  
e.g.,

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \sum_{j=3}^M \theta_j (x - \xi_j)_+^2$$

- P-splines and smoothing splines are **”typically” equivalent**, even for  $M = 15$ , at least in our context
- We place knots at quantiles of the  $W$ -distribution

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## MEAN-BASED STRUCTURAL METHODS

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$$m(x) = \sum_{j=1}^M \theta_j B_j(x)$$

- It follows that

$$E(Y|W) = \sum_{j=1}^M \theta_j E\{B_j(X)|W\} = \sum_{j=1}^M \theta_j Q_j(W)$$

- If  $X$  is parametric, and  $U$  is normal, then  $[X|W]$  is known and  $Q_j(\cdot)$  is readily calculated

- **Penalization:** for some matrix  $D$ , minimize

$$\sum_{i=1}^n \{Y_i - \sum_{j=1}^M \theta_j Q_j(W)\}^2 + \alpha \underline{\theta}^T D \underline{\theta}$$

- **Ridge-type estimator:**  $\alpha$  must be estimated

- Shrinkage of  $B_j$  to  $W \implies Q_j$  **nearly singular**
- $\alpha = 0$  yields **enormously variable estimates**
- We developed a “**minimize estimated MSE**” shrinkage method

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## SPLINES: FULLY STRUCTURAL

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- If we specify a distribution for  $X$  and  $\epsilon$ , then we have a **fully specified parametric model** using the standard mixed model formulation:

$$Y = \theta_0 + \theta_1 x + \theta_2 x^2 + \sum_{j=3}^M \theta_j (x - \xi_j)_+^2 + \epsilon$$

$$\theta_j = \text{Normal}(0, \sigma_\theta^2) \text{ for } j \geq 3$$

$$\epsilon = \text{Normal}(0, \sigma_\epsilon^2)$$

$$X = \text{Normal}(\mu_x, \sigma_x^2)$$

$$W = \text{Normal}(X, \sigma_u^2)$$

- Good starting values are easy: previous method or SIMEX
- A penalty is incorporated naturally through the variance component  $\sigma_\theta^2$
- Computed via MCMC: program on my web site

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## COMMENTS ON FULLY STRUCTURAL

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- We have investigated allowing  $X$  to have a flexible distribution, i.e., mixture of  $\leq 3$  normals
- More complex computationally
- Useful for severely skew  $X$ , not much gain otherwise (or loss!)
- Still, **structural spline is remarkably robust to deviations from normality for  $X$**

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## SPECIAL CASE: SIMULATION

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- $n = 200$  with

$$m(x) = \frac{\sin(\pi x/2)}{1 + 2x^2\{\text{sign}(x) + 1\}}$$

- $X$  standard normal, 30% of observed variability in  $W$  due to error
- Frequentist MSE
  - Naive smoothing spline: 5.6
  - SIMEX smoothing spline: 4.7
  - Mean-based P-spline,  $M = 15$ : 3.8
  - Bayes P-spline,  $M = 40$ : 1.6
- Note: **Bayes method is a better frequentist estimator**
- Here are some examples for  $\sin(2x)$  with different amounts of measurement error

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## SIMEX

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- As I will show via simulated data, the naive estimate in the presence of measurement error **loses all features**
- That is, with sufficiently large measurement error, the  $Y$  and  $W$  data look like a polynomial
- The SIMEX method can be expected to perform fairly poorly here.
- SIMEX adds error to a problem that has already lost its features
- Each SIMEX step is going to fit a polynomial
- Thus, SIMEX with sufficiently large measurement error is typically going to be a corrected polynomial fit.

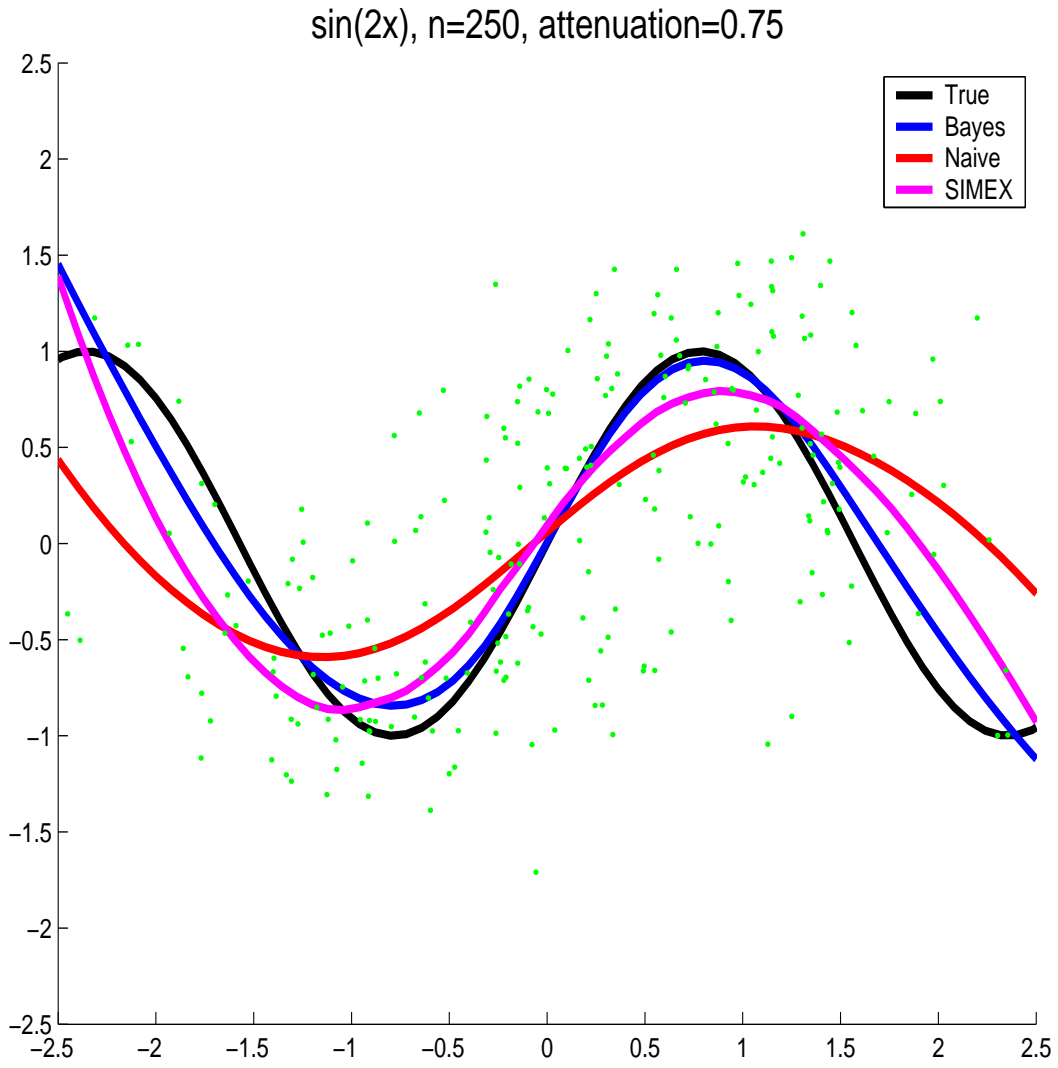


Figure 1: Note how the naive fit captures some of the features, so SIMEX does much better

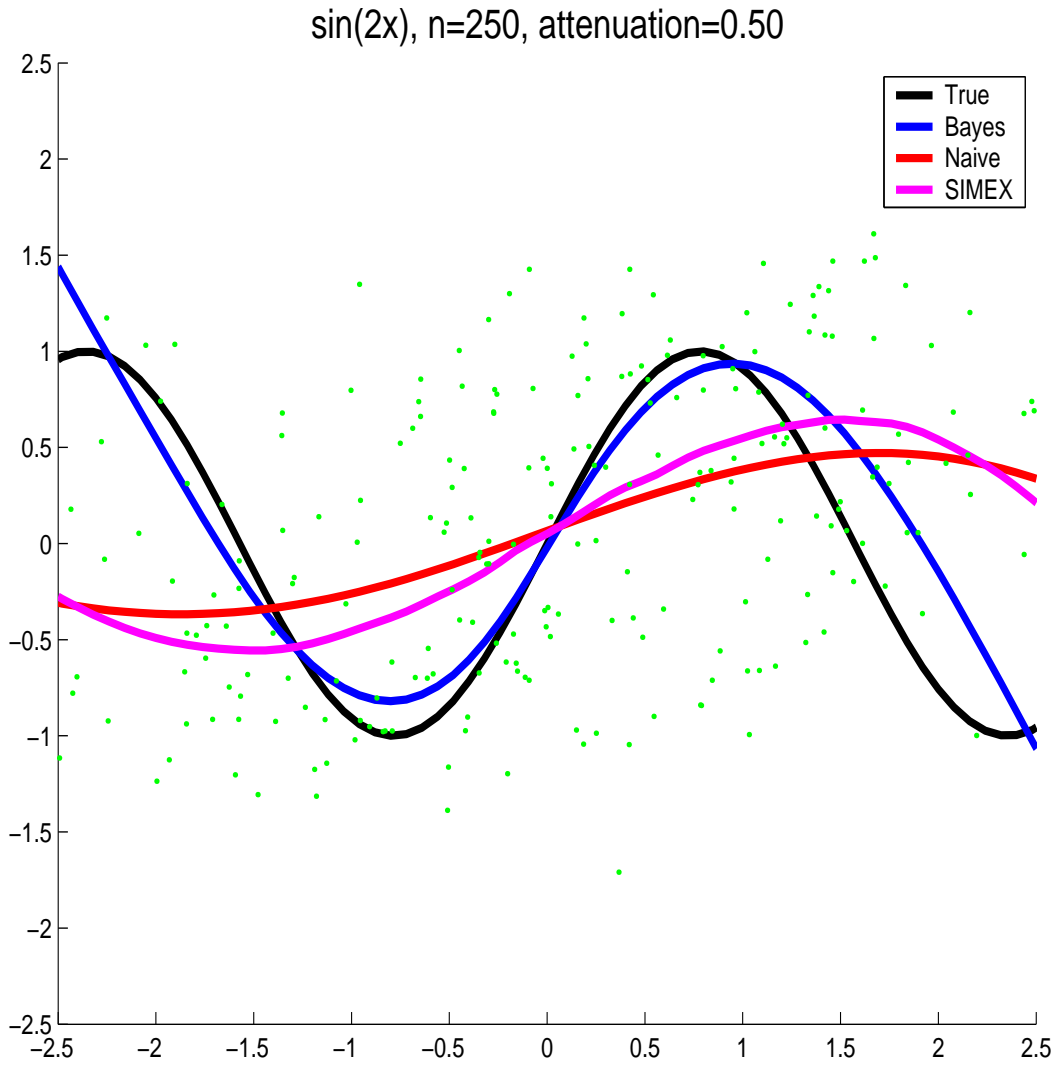
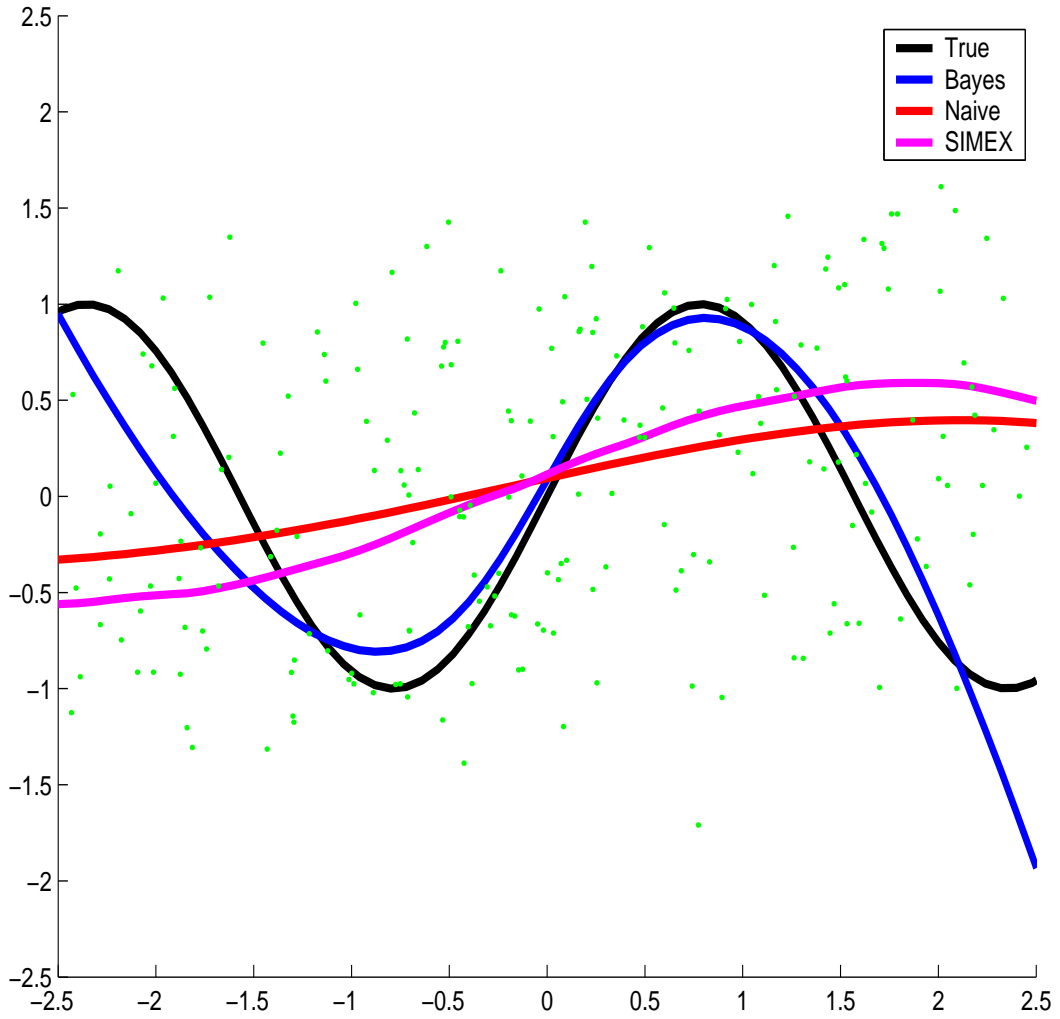


Figure 2: Note how the naive fit captures **NONE** of the features, so SIMEX does **NO** better

$\sin(2x)$ ,  $n=250$ , attenuation=0.33



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## WHY DOES THE STRUCTURAL SPLINE WORK SO WELL?

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- Take  $m(x) = \sin(2x)$ ,  $X \sim \text{Normal}(1, 1)$ ,  $\lambda = 2/3$ ,  $\sigma_\epsilon^2 = 0.15$ .
- Estimate  $X$ 
  - Estimate #1:  $E(X|W)$
  - Estimate #2: Mean of  $X$  over MCMC samples
- Ratio of MSE for  $\sin(2\hat{X}) \approx 3$
- Structural spline with MCMC gives a **much** better estimate of  $X$
- Structural Spline with MCMC uses the assumed distribution of  $Y$  given  $X$  in a strong way
- Suggests **potential** for model non-robustness

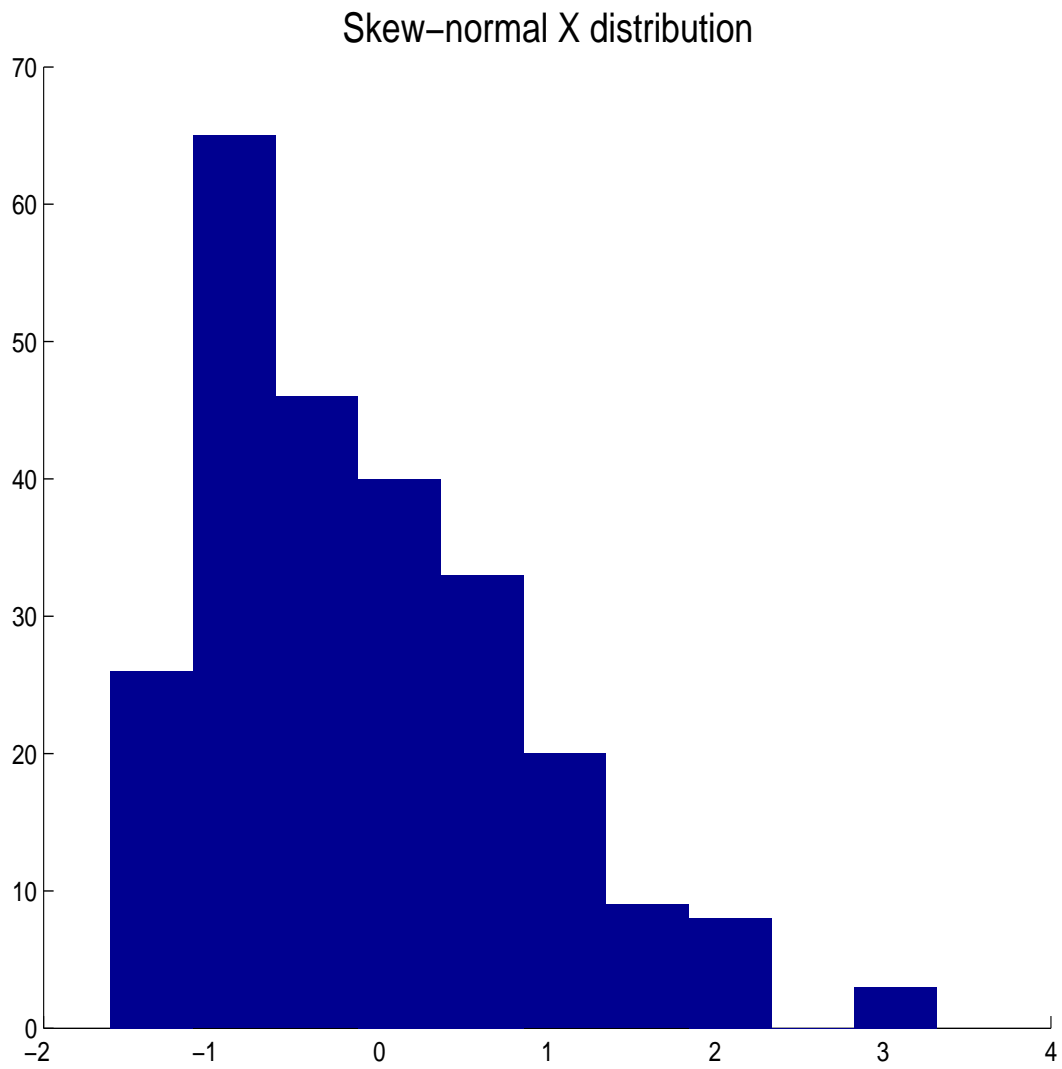


Figure 3: This is the distribution for  $X$  and  $\epsilon$ , which are both **assumed** to be normal

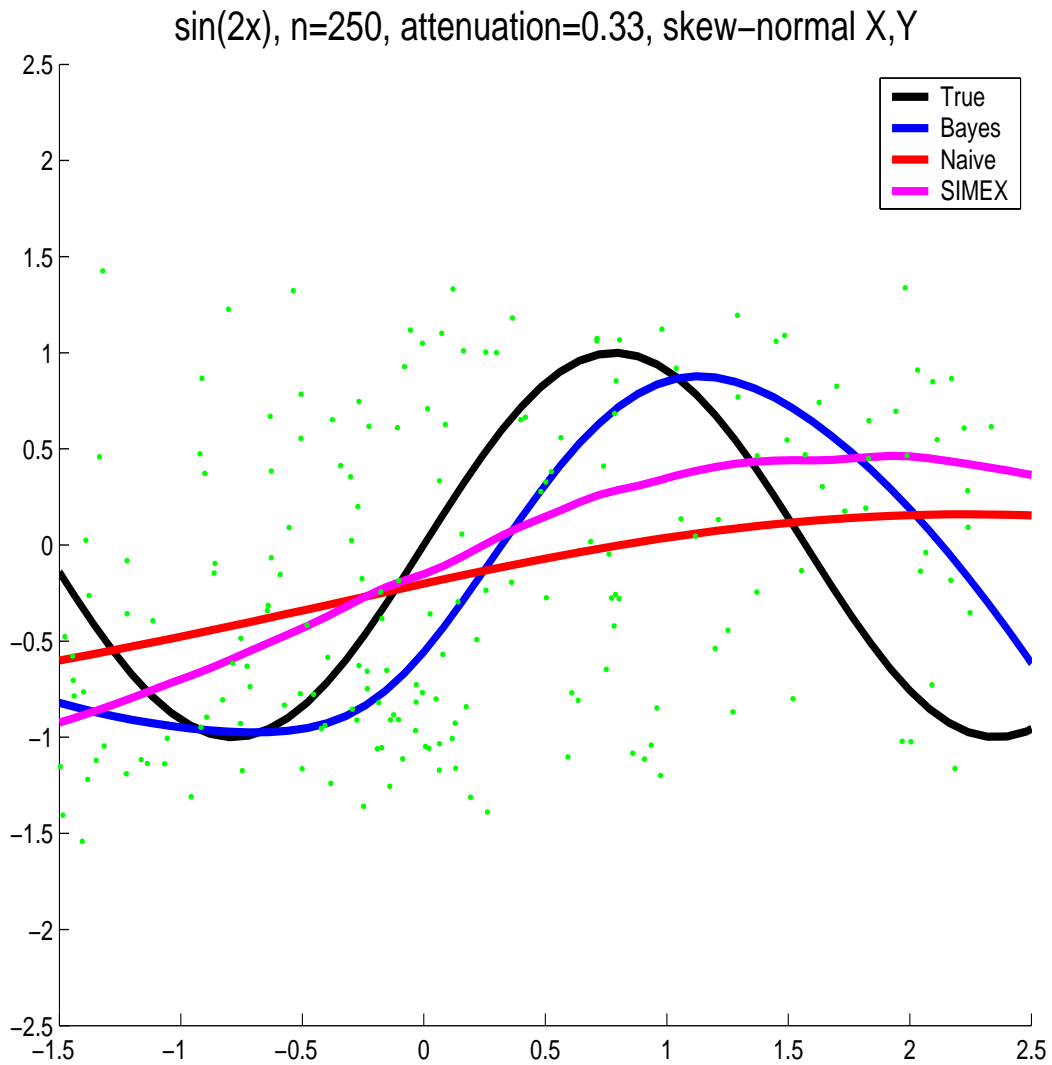


Figure 4: Here you assume that  $X$  and  $\epsilon$  are normal, when they are skew-normal. Note how the Bayes fit is still much better than naive or SIMEX, but clearly worse than the normal  $X$  and  $\epsilon$  simulation

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## SUMMARY OF METHODS

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- **Naive**: great estimate of the wrong thing
- **Deconvolution**: lousy estimate of the right thing
- **SIMEX**: approximately consistent, no assumptions, **cannot cope with large measurement error**
- **Mean function** P-splines
  - Parametric model for  $[X]$
  - Flexible mean function
  - **Ad hoc smoothing**
- **Structural splines**
  - Parametric model for  $Y$  given  $X$ ,  $[X]$
  - MCMC incorporates penalty naturally
  - Results great even when  $X \sim \chi^2(4)$
  - **Few** results yet when  $Y$  given  $X$  is mismodeled

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## CONCLUSIONS

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- The more (correct!) assumptions you make, the more efficient the estimator
- Hierarchy
  - Global consistency,  $[X]$ ,  $Y$  given  $X$  unspecified
  - Approximate consistency,  $[X]$ ,  $Y$  given  $X$  unspecified
  - Flexible means,  $[X]$  specified
  - Bayes,  $[X]$ ,  $Y$  given  $X$  specified
- **It is remarkable** how well you can extract the features of the problem in the presence of measurement error