Chaos, Complexity, and Inference (36-462)

Lecture 4

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22 January 2009

Reconstruction Inferring the attractor from a time series; powerful in a weird way

Prediction Using the reconstructed attractor to make forecasts

Reconstruction

What can we learn about the dynamical system from observing a trajectory?

Assume it's reached an attractor; attractor is a function of the parameters; invert the function

- Function from parameters to attractors can be very ugly
- Assumes we know the dynamics up to parameters

Second problem is bigger!

Will see later an approach ("indirect inference") for parametric estimation with messy models

Do we need parameters?

A gross simplification of

Takens's Embedding Theorem

Suppose X_t is a state vector
Suppose the map/flow is sufficiently smooth
Suppose X_t has gone to an attractor, dimension d
Suppose we observe $S_t = g(X_t)$, which again is sufficiently smooth
Pick a time-lag τ and a number of lags k
Time-delay vector $R_t^{(k)} = (S_t, S_{t-\tau}, S_{t-2\tau}, \ldots S_{t-(k-1)\tau})$
THEOREM If $k \geq 2d + 1$, then, for generic g and τ, $R_t^{(k)}$ acts just like X_t, up to a smooth change of coordinates

Determinism

State has d dimensions so knowing d coordinates at once fixes trajectory
OR knowing one variable at d times fixes trajectory (think of Henon map)
Don't get to observe state variables so may need extra observations
Turn out to never need more than $d + 1$ extras
Sometimes don't need the extras
[Packard et al., 1980]

Geometry

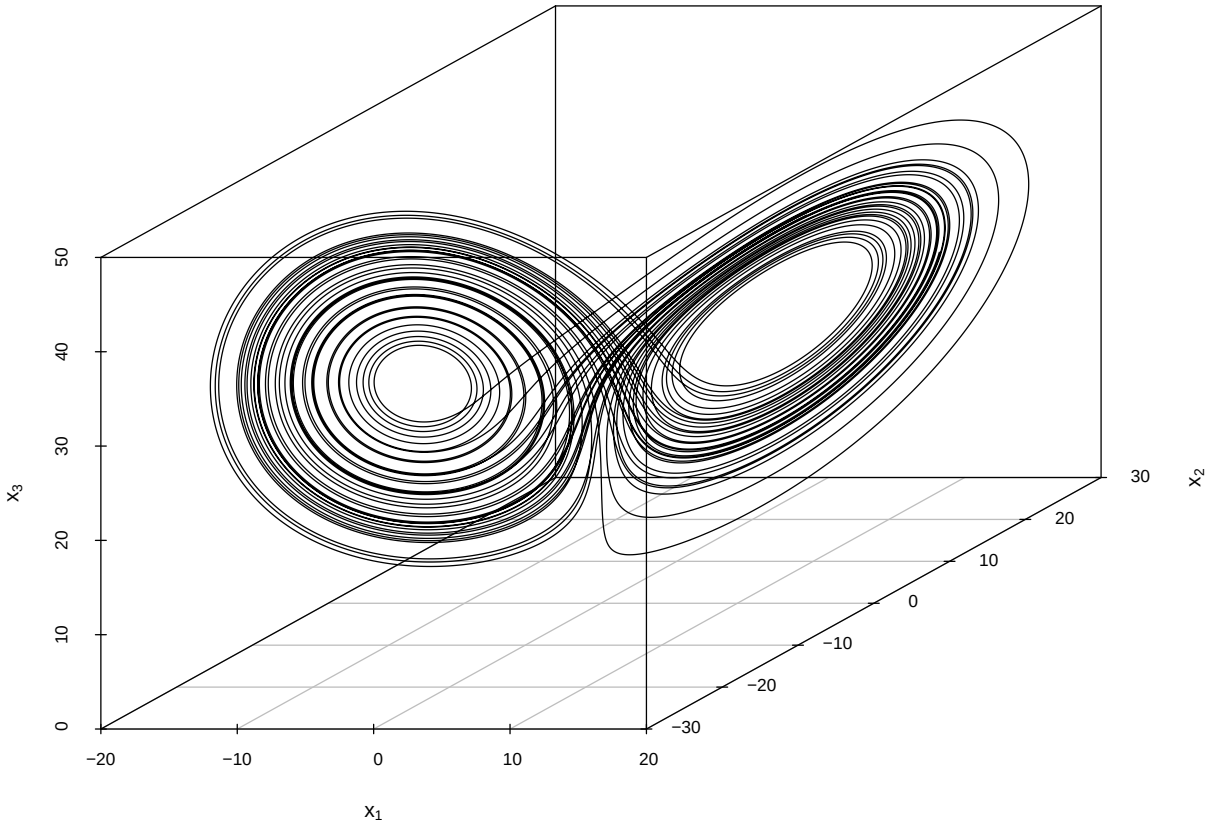
Trajectories are d-dimensional (because they are on the attractor, and current state fixes future states)
So time series are also only d-dimensional, but they might live on a weirdly curved d-dimensional space
Geometric fact (Whitney embedding theorem): any curved d-dimensional space fits into a $2d + 1$-dimensional ordinary Euclidean space
[Takens, 1981]

An example of reconstruction

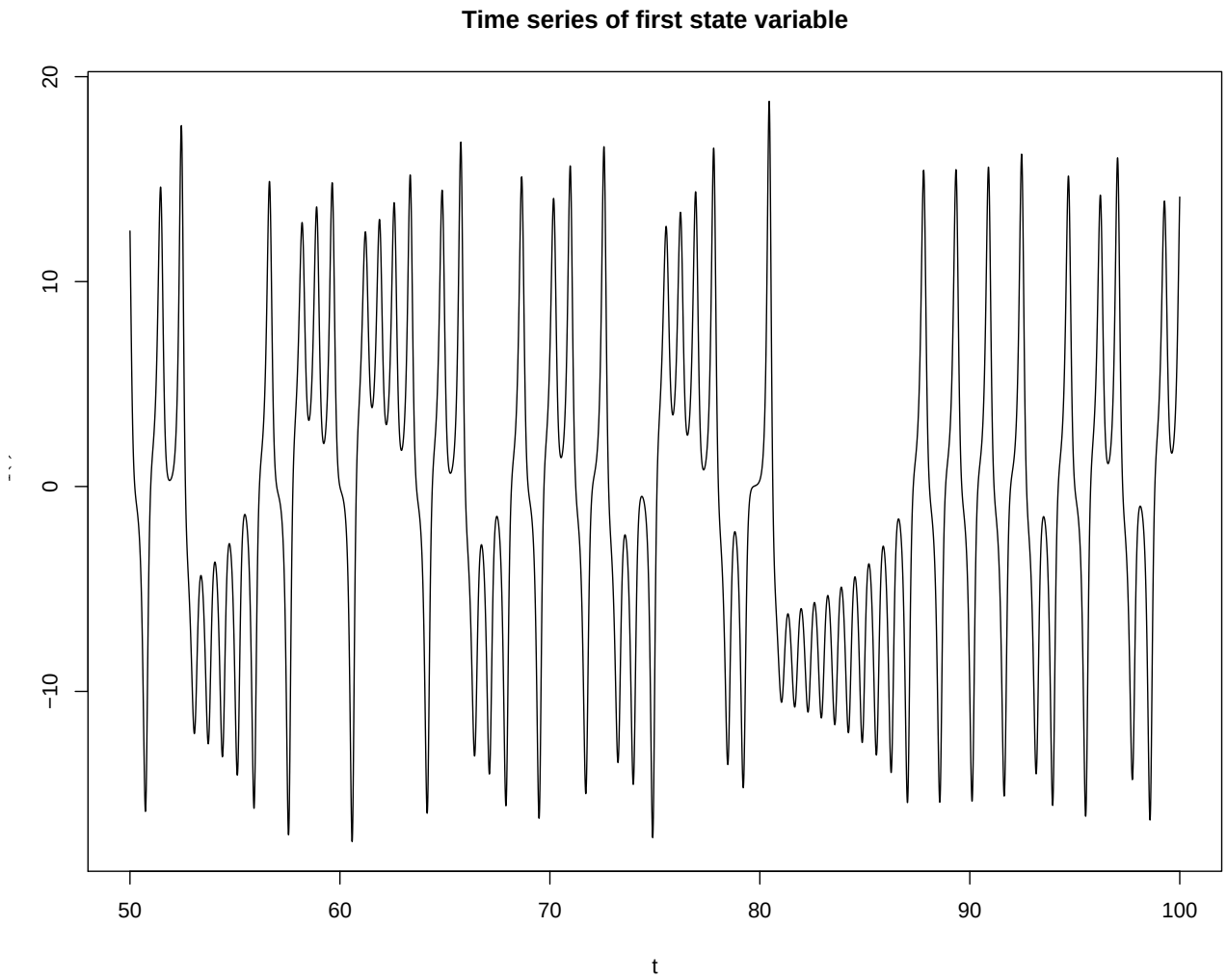
Lorenz attractor, $a = 10$, $b = 28$, $c = 8/3$
See last lecture for equations of motion
Solved equations in a separate (non-R) program (see website)

```
> lorenz.state.ts = read.csv("lorenz-t50-to-t100-by-1e-3",
                             col.names=c("t","x","y","z"))
> scatterplot3d(lorenz.state.ts$x,lorenz.state.ts$y,
                lorenz.state.ts$z,type="l",xlab="x",
                ylab="y",zlab="z",lwd="0.2")
> x.ts = lorenz.state.ts$x
> library(tseriesChaos)
> scatterplot3d(embedd(x.ts,3,40),type="l",lwd="0.2")
```

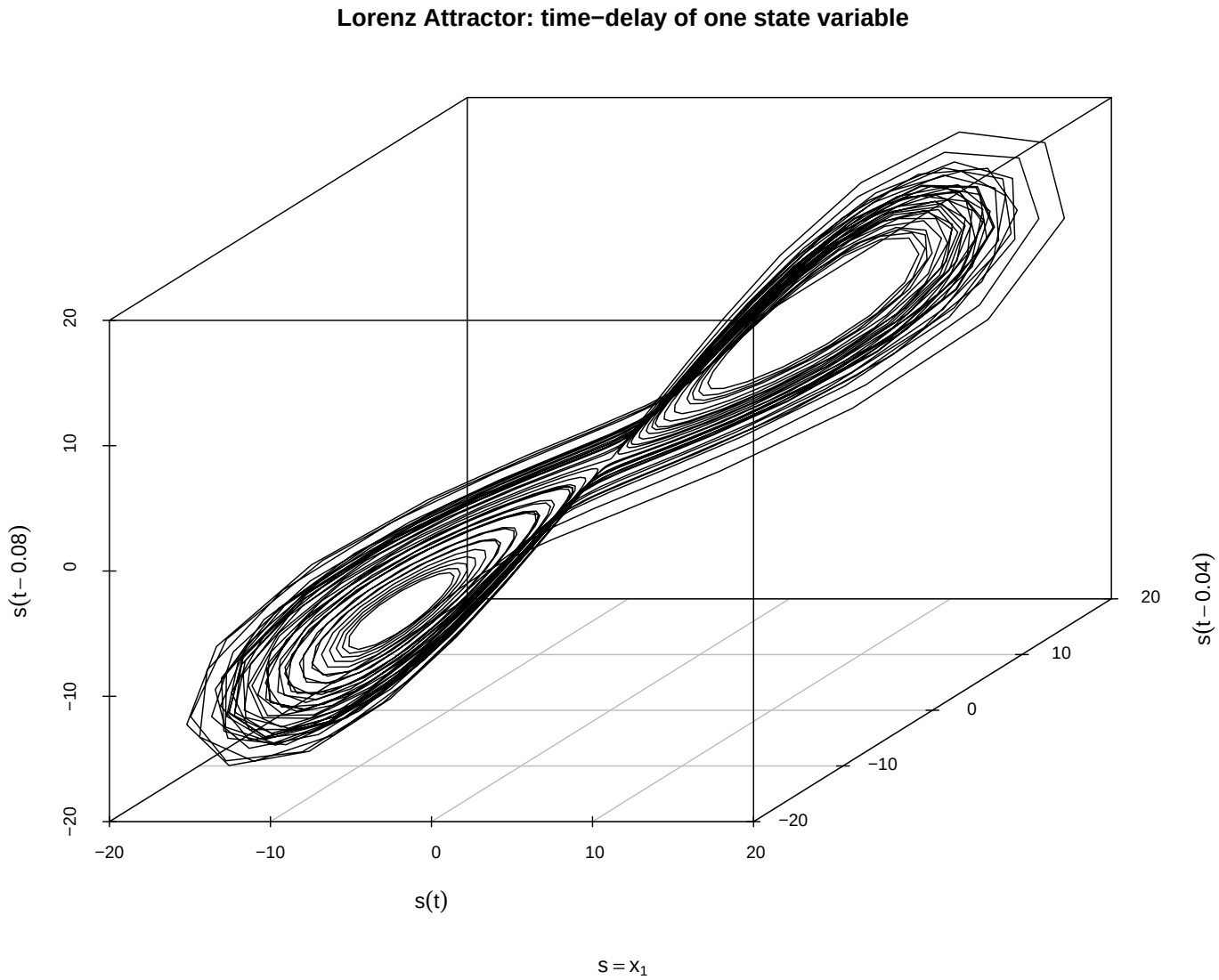
Lorenz Attractor: state space

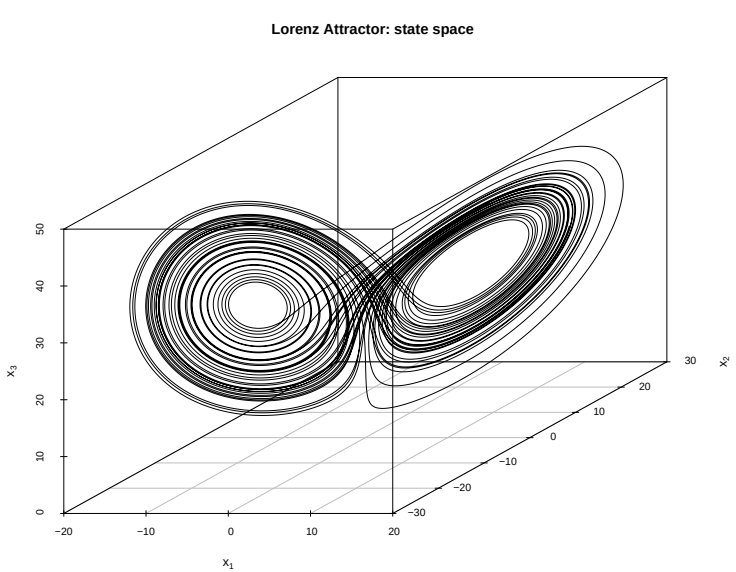


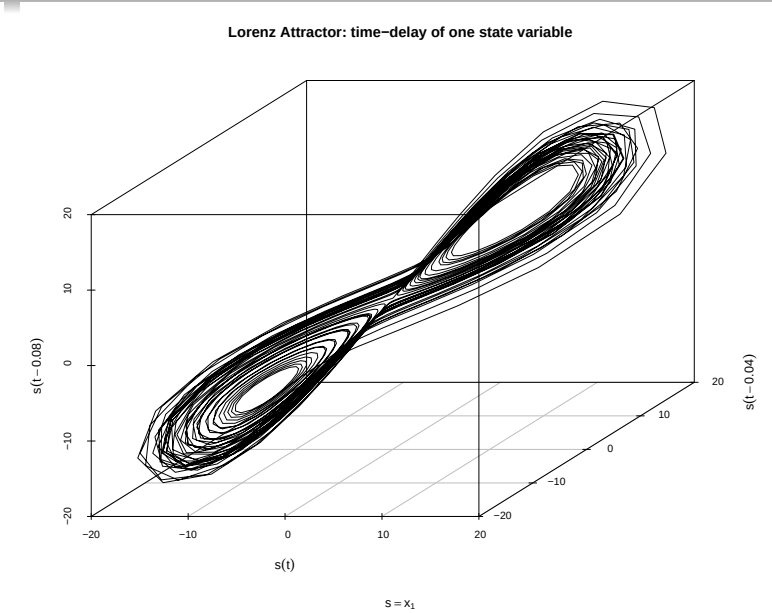
Time series: first coordinate of state



Reconstruction, $k = 3$, $\tau = 0.04$







Note: reconstruction procedure knew nothing about what the state variables were or what the equations of motion were, it just worked with the original time-series

Attractor Reconstruction

"It's inference, Jim, but not as we know it"
Gets information about the larger system generating the data from partial data (inference)
No parametric model form
No nonparametric model form either
No likelihood, no prior
Requires very complete determinism
Reconstructs the attractor up to a smooth change of coordinates

Coordinate change

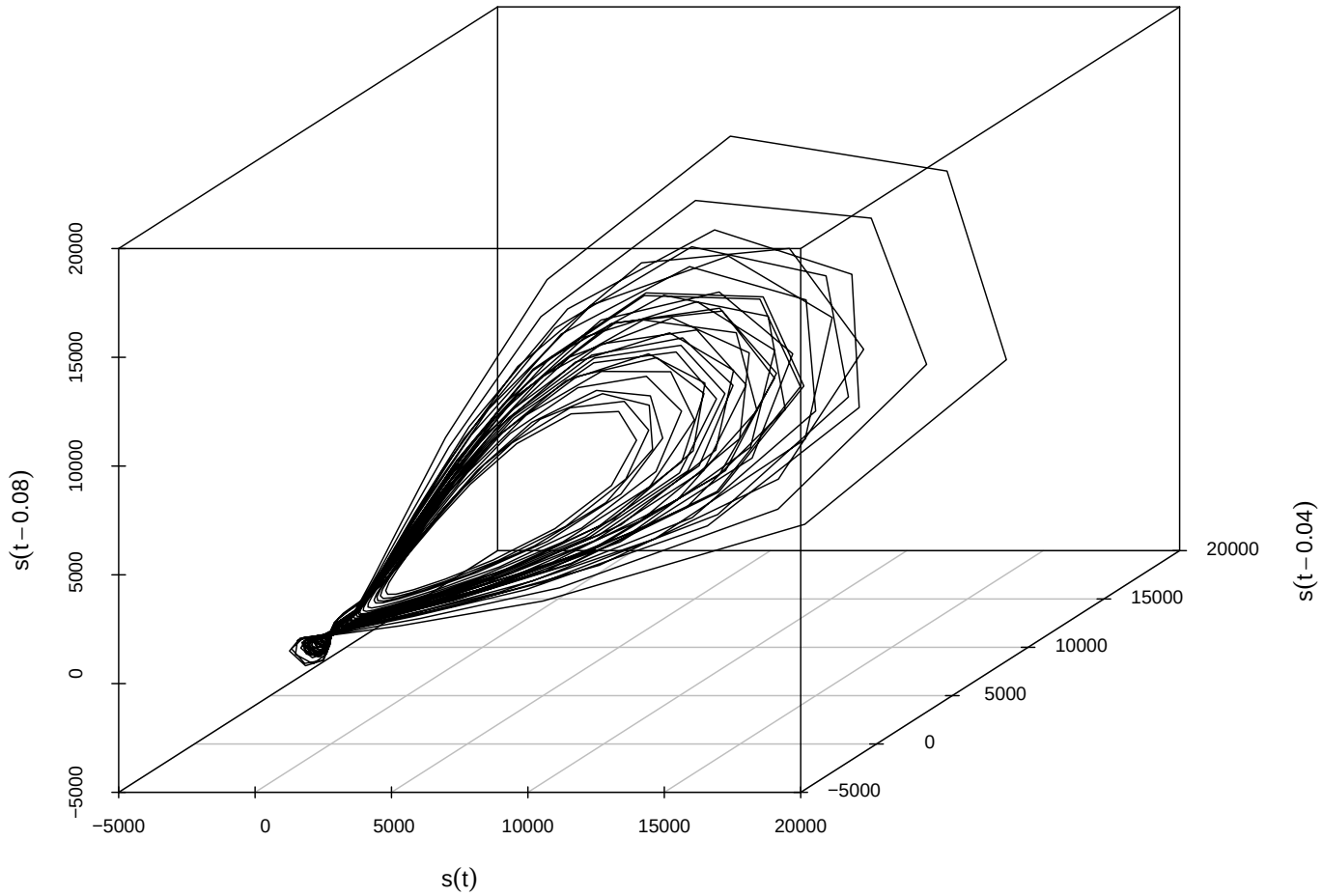
old, new state $= X_t$, R_t
old, new map $= \Phi$, Ψ
coordinate change $= G$ so $R_t = G(X_t)$
If the coordinate change works, then it doesn't matter whether we apply it or the map first

$$\begin{aligned} X_{t+1} = \Phi(X_t) \qquad & R_{t+1} = \Psi(R_t) \\ R_{t+1} = G(\Phi(X_t)) \quad = \quad & \Psi(G(X_t)) = R_{t+1} \end{aligned}$$

$$\begin{array}{ccc} X_t & \xrightarrow{\Phi} & X_{t+1} \\ G \downarrow & & G \downarrow \\ R_t & \xrightarrow{\Psi} & R_{t+1} \end{array}$$

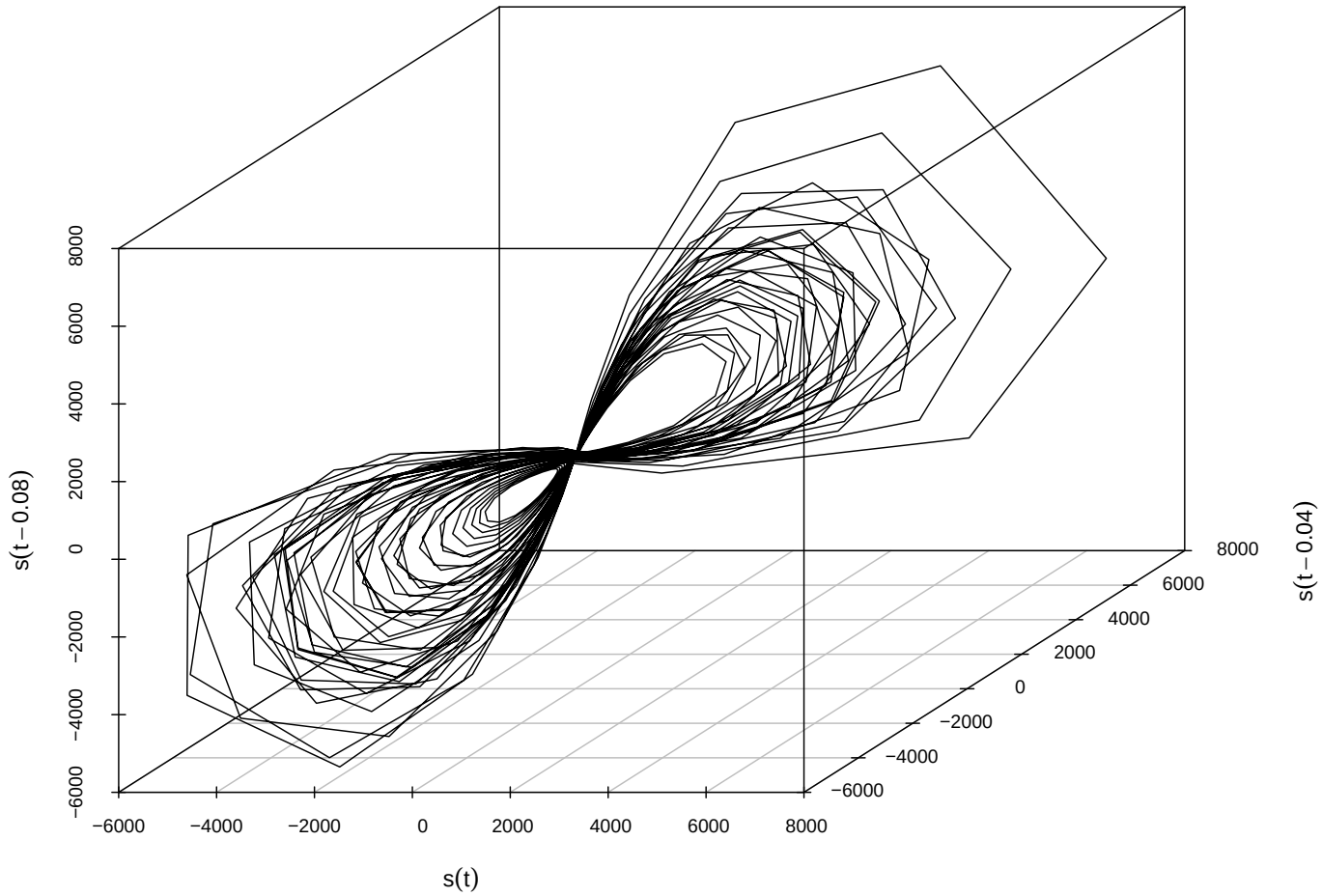
New coordinates are a perfect model of the old coordinates
time-delay vectors give a model of states, at least on the attractor
many quantities (like Lyapunov exponents) aren't affected by change of coordinates

Lorenz Attractor: nonlinear observable



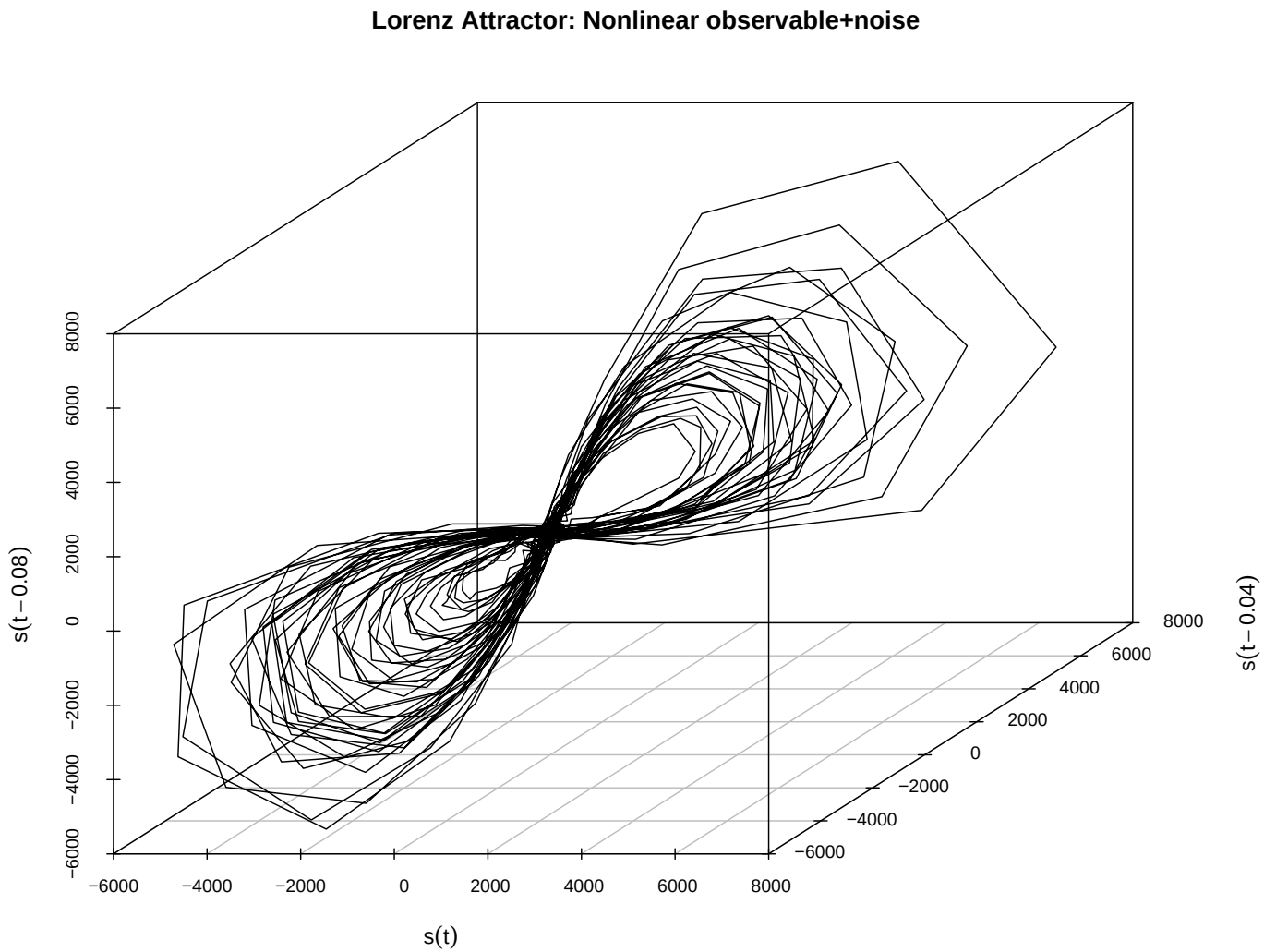
$$s = (x_1 + 7)^3$$

Lorenz Attractor: Nonlinear observable



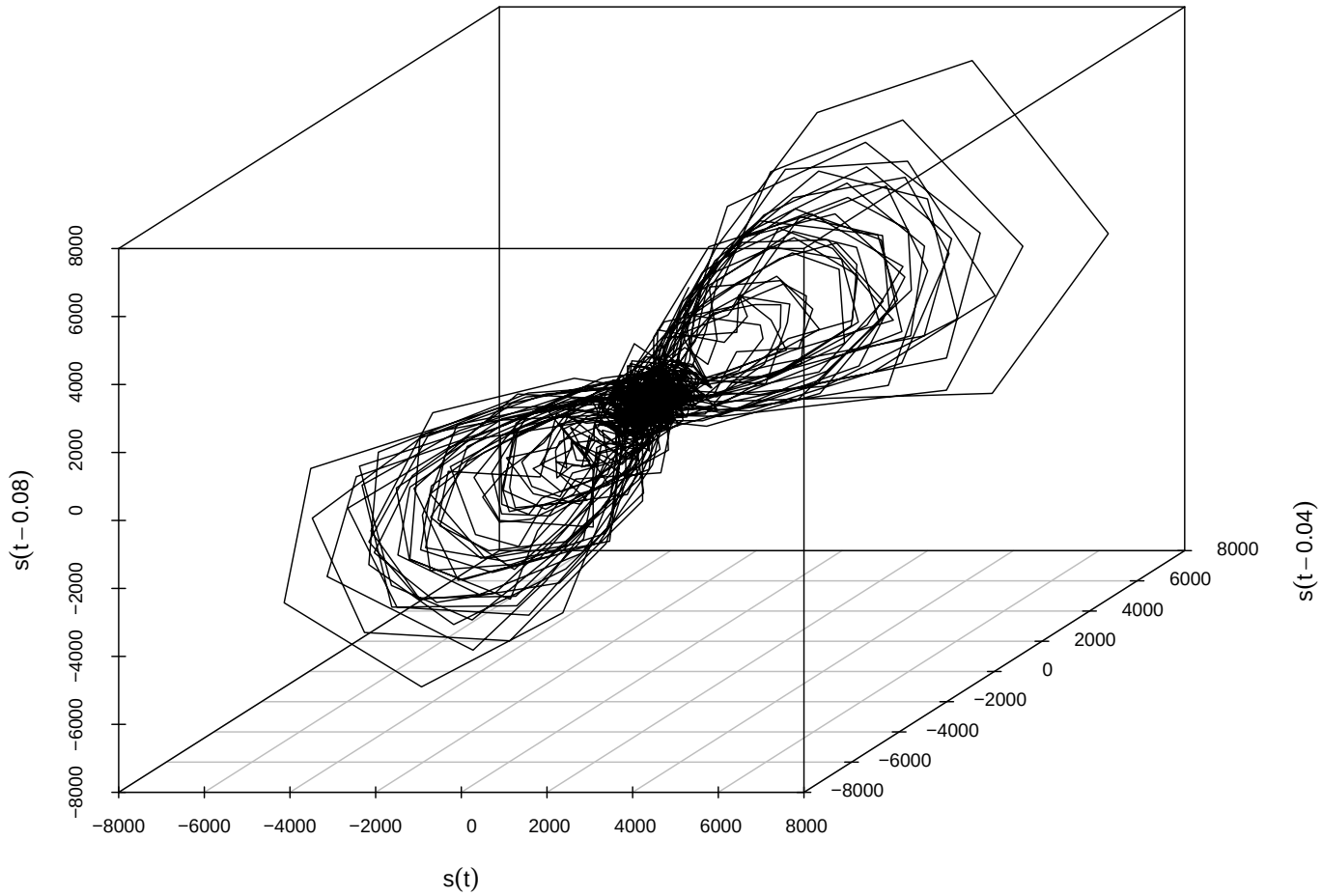
$s = x_1^2 x_2$

It even works with observation noise



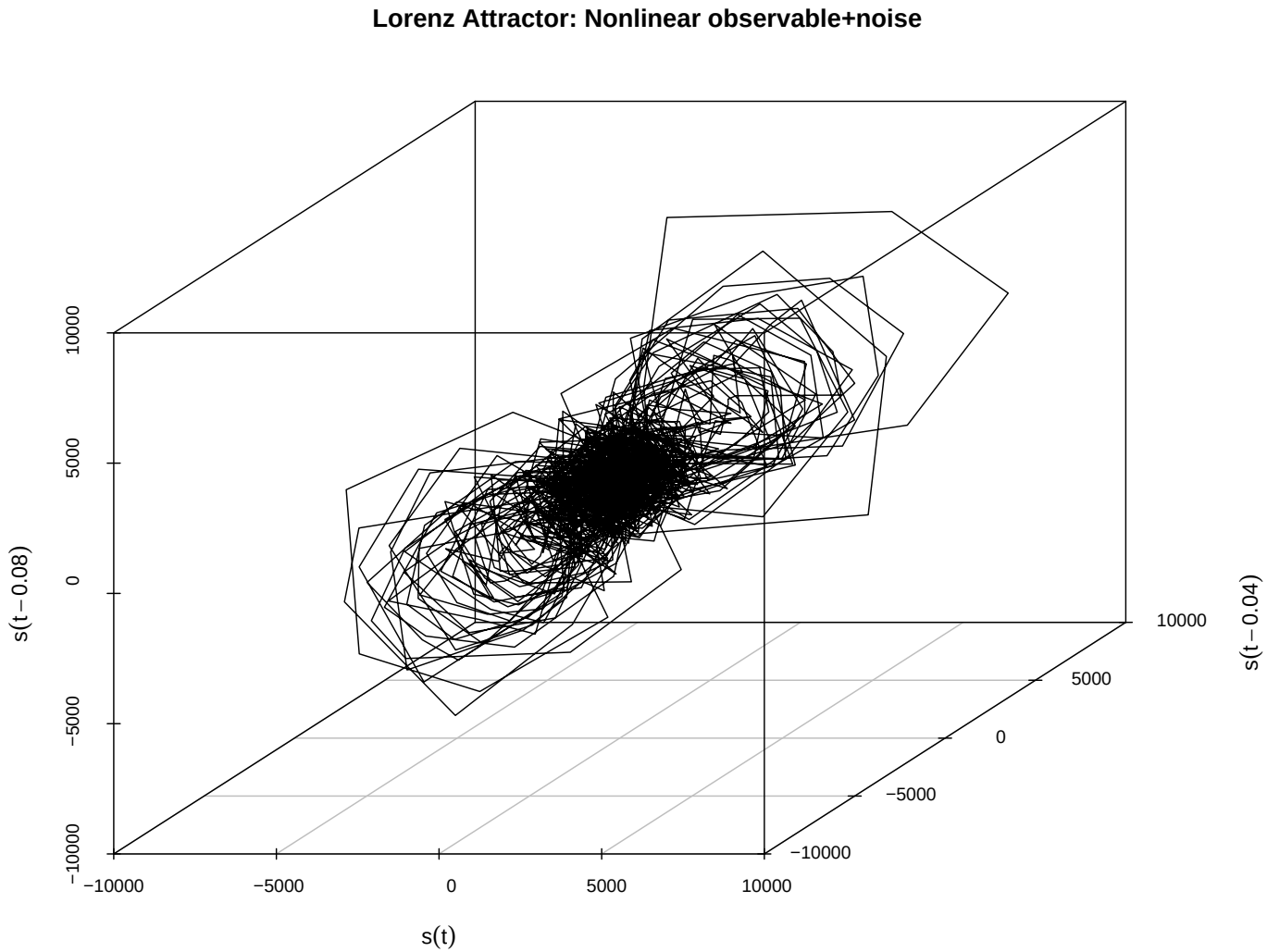
$s = x_1^2 x_2 + \varepsilon,\ \sigma(\varepsilon) = 100$

Lorenz Attractor: Nonlinear observable+noise



$s = x_1^2 x_2 + \varepsilon,\ \sigma(\varepsilon) = 400$

but not too much



$s = x_1^2 x_2 + \varepsilon,\ \sigma(\varepsilon) = 1000$

Choice of reconstruction settings

Need to choose k (number of delays, embedding dimension) and τ (delay between observations) — typically the observable is given to us by the problem situation
These involve a certain amount of uncertainty
Software: used `tseriesChaos` from CRAN
Hegger, Kantz, & Schreiber's TISEAN has an R port, `RTisean`, also on CRAN, couldn't get it to work

Choice of delay τ

In principle, almost any τ will do

but if the attractor is periodic, multiples of the period are bad!

In practice, want to try and get as much new information about the state as possible from each observation

$\Rightarrow$ Heuristic 1: make τ the first minimum of the autocorrelation

$\Rightarrow$ Heuristic 2: make τ the first minimum of the mutual information

Will return to heuristic 2 after we explain “mutual information”

Autocorrelation function

$$\rho(t,s) = \frac{\mathrm{cov}[X_t, X_s]}{\sigma(X_t)\sigma(X_s)}$$

For **weakly stationary** or **second-order stationary** processes, $\rho(t,s) = \rho(|t-s|)$, i.e., depends only on time-lag, not on absolute time

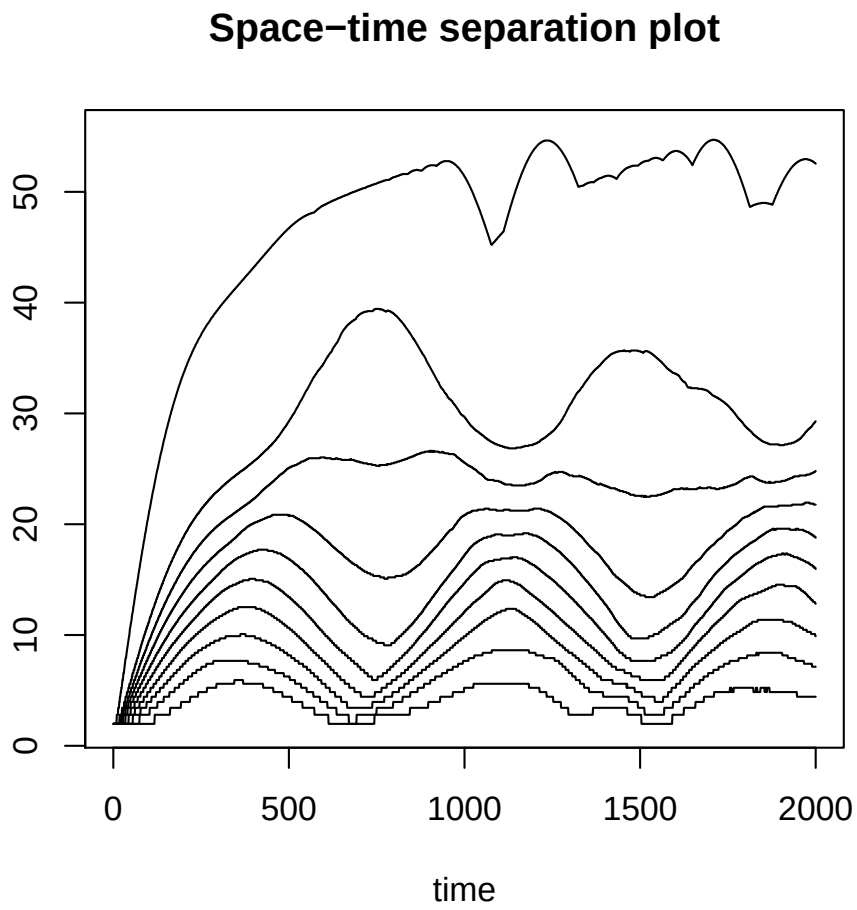
Standard `R` command: `acf`

Space-time separation plot

Distance between two random points from the trajectory will depend on how far apart in time we make the observations
For each $h > 0$, calculate the empirical distribution of $\|X_t - Y_{t+h}\|$
Plot the quantiles as a function of h
Example: logistic map

```
stplot(x.ts,3,40,mdt=2000)
```

showing deciles; time in units of $1/1000$

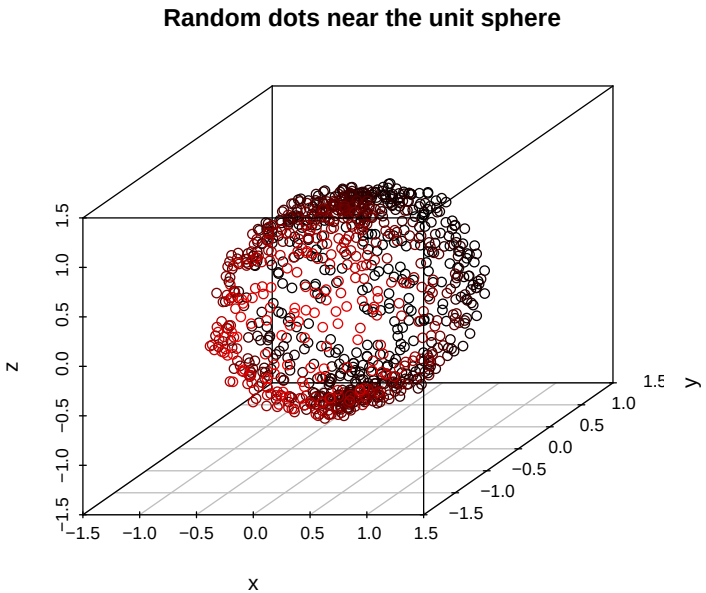


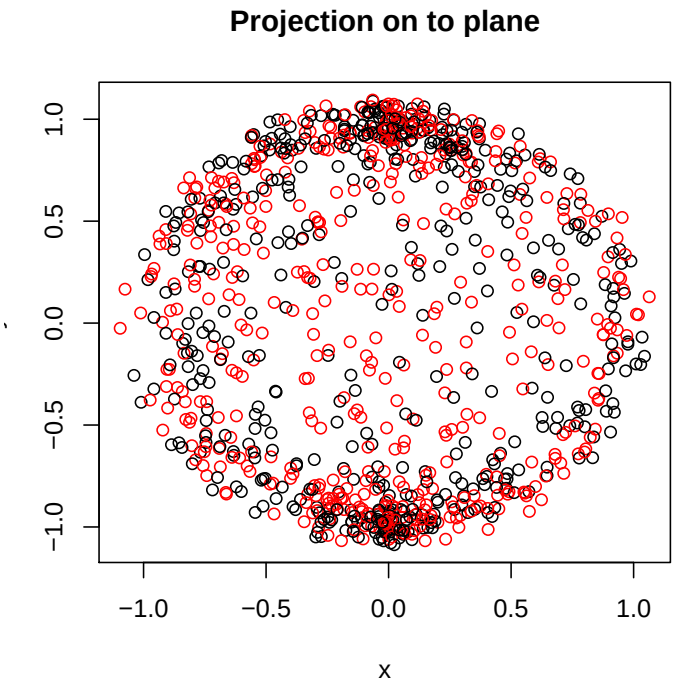
note growth (separation) + periodicity

correlations are reasonably decayed at around ≈ 250, before then observatons are correlated because not enough time to disperse around attractor

Choice of embedding dimension k: False Neighbor Method

Take points which really live in a high-dimensional space and project into a low-dimensional one: many points which are really far apart will have projections which are close by
These are the **false neighbors**



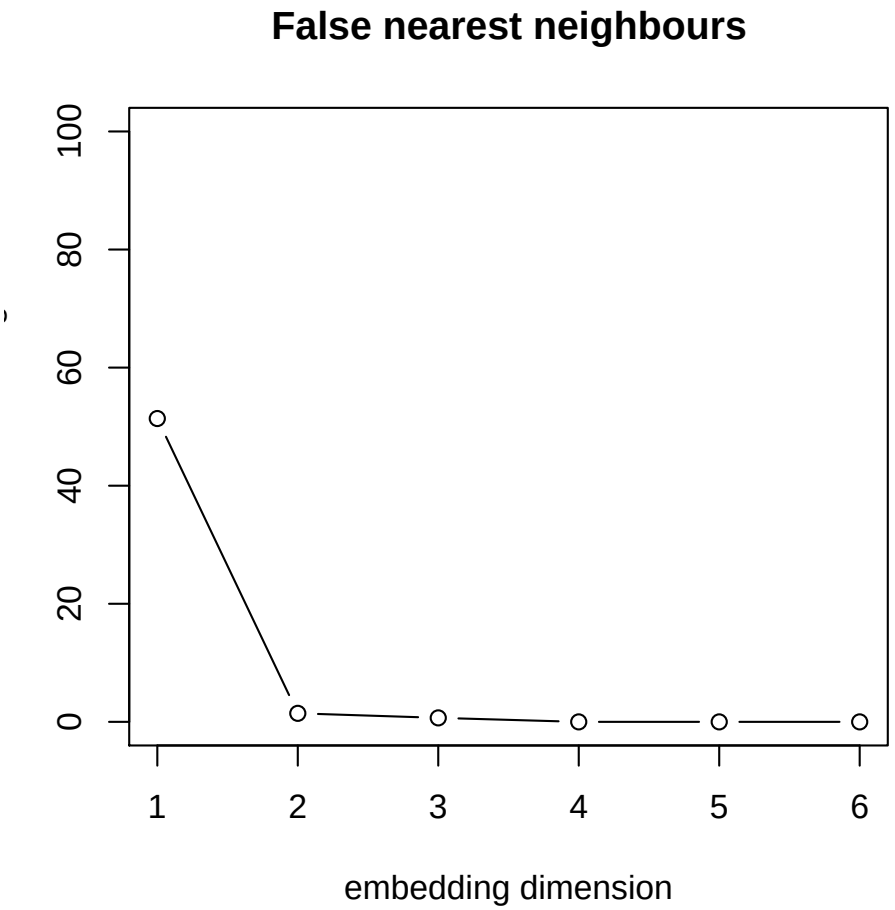


Keep increasing the dimensionality until everything which was a neighbor in k dimensions is still a neighbor in $k + 1$ dimensions

Need to exclude points which are nearby just because the dynamics hasn't had time to separate them — calculate this **Theiler window** from space-time plot

```
plot(false.nearest(x.ts,6,40,250))
```

i.e. use $\tau = 40$ in embedding, consider up to 6 dimensions, and use an Theiler exclusion window of 250 time-steps



Conclusion: $k = 3$ it is

Prediction

Determinism: there is a mapping from old states to new states
Prediction: learn that mapping, then apply it
Work in the reconstructed state space

Nearest-neighbor methods

Also called **method of analogs** in dynamics
Given: points $x_1, x_2, x_3, \ldots x_{n-1}$ and their sequels, $x_2, x_3, \ldots x_n$
Wanted: prediction of what will happen after seeing new point x
Nearest neighbor: find x_i closest to x; predict x_{i+1}
k**-nearest neighbors**: find k points $x_{i_1}, x_{i_2}, x_{i_k}$ closest to x, predict the average of $x_{i_1+1}, x_{i_2+1}, \ldots x_{i_k+1}$
Notation: $U_k(x) = k$ nearest neighbors of x
Note: this k is not the k of the embedding dimension, but the phrase "k-nearest neighbors" is traditional
Computation: finding the nearest neighbors fast is tricky; leave it to a professional

Assume the map Φ is smooth
If x_i is very close to x, then $\Phi(x_i) = x_{i+1}$ will be close to, but not exactly, $\Phi(x)$

$$\Phi(x_i) = \Phi(x) + (x_i - x)\Phi'(x) + \text{small}$$

If $x_{i_1}, x_{i_2}, x_{i_k}$ are all very close to x, then $x_{i_1+1}, x_{i_2+1}, \ldots x_{i_k+1}$ should all be close to $\Phi(x)$

$$\frac{1}{k}\sum_{j\in U_k(x)}\Phi(x_j) = \frac{1}{k}\sum_{j\in U_k(x)}\Phi(x) + \left(\frac{1}{k}\sum_{j\in U_k(x)} x_j - x\right)\Phi'(x) + \text{small}$$

$$\frac{1}{k}\sum_{j\in U_k(x)}\Phi(x_j) - \Phi(x) \approx \left(\frac{1}{k}\sum_{j\in U_k(x)} x_j - x\right)\Phi'(x)$$

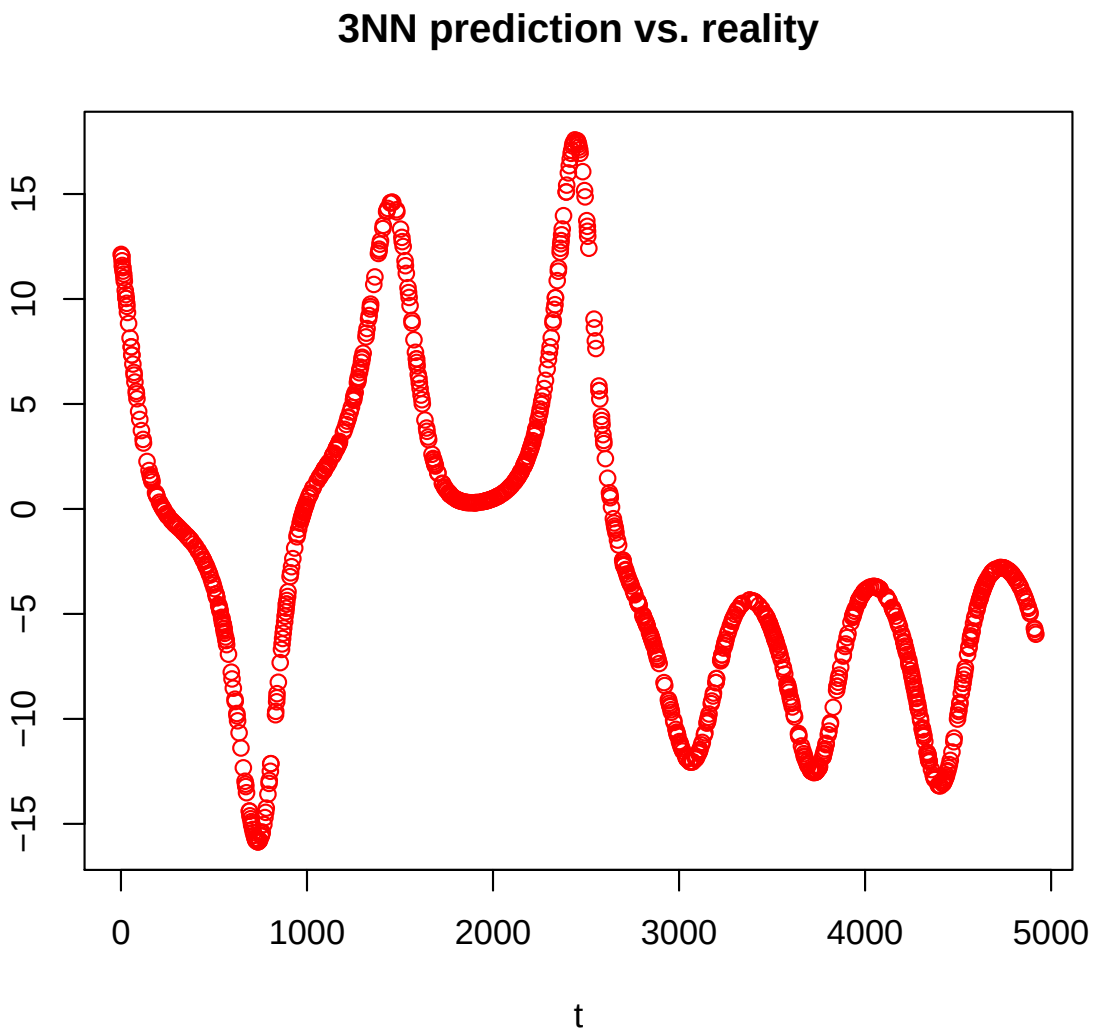
$k > 1$: the error averages a bunch of individual terms from the neighbors, which should tend to be smaller than any one of them, *if* they're not too correlated themselves
One reason this works well together with mixing!

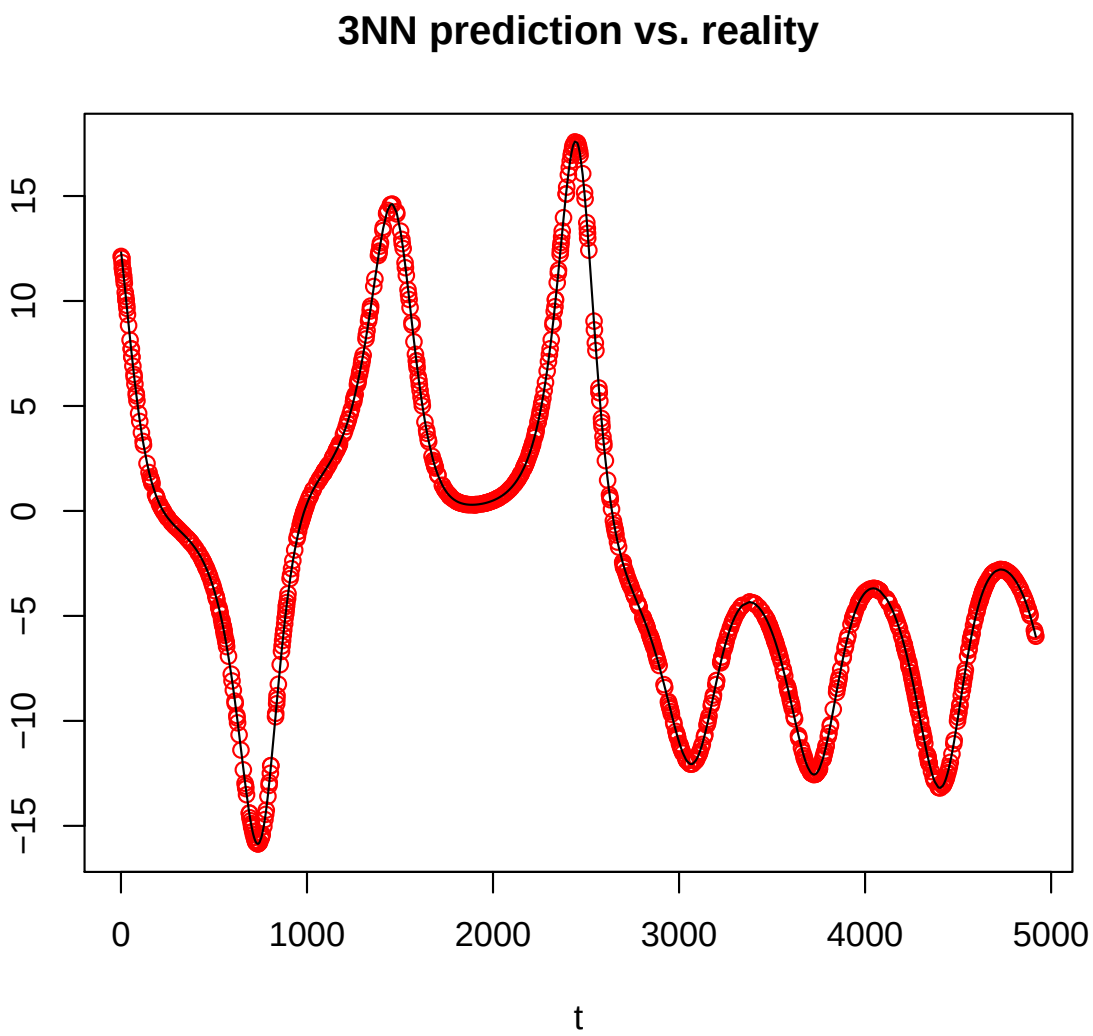
As n grows, we get more and more samples along the attractor
If x itself is from the attractor, it becomes more and more likely that we are sampling from a place where we have many neighbors, and hence close neighbors, so the accuracy should keep going up
Another reason this works well with mixing

`knnflex` from CRAN lets you do nearest-neighbor prediction (as well as classification)

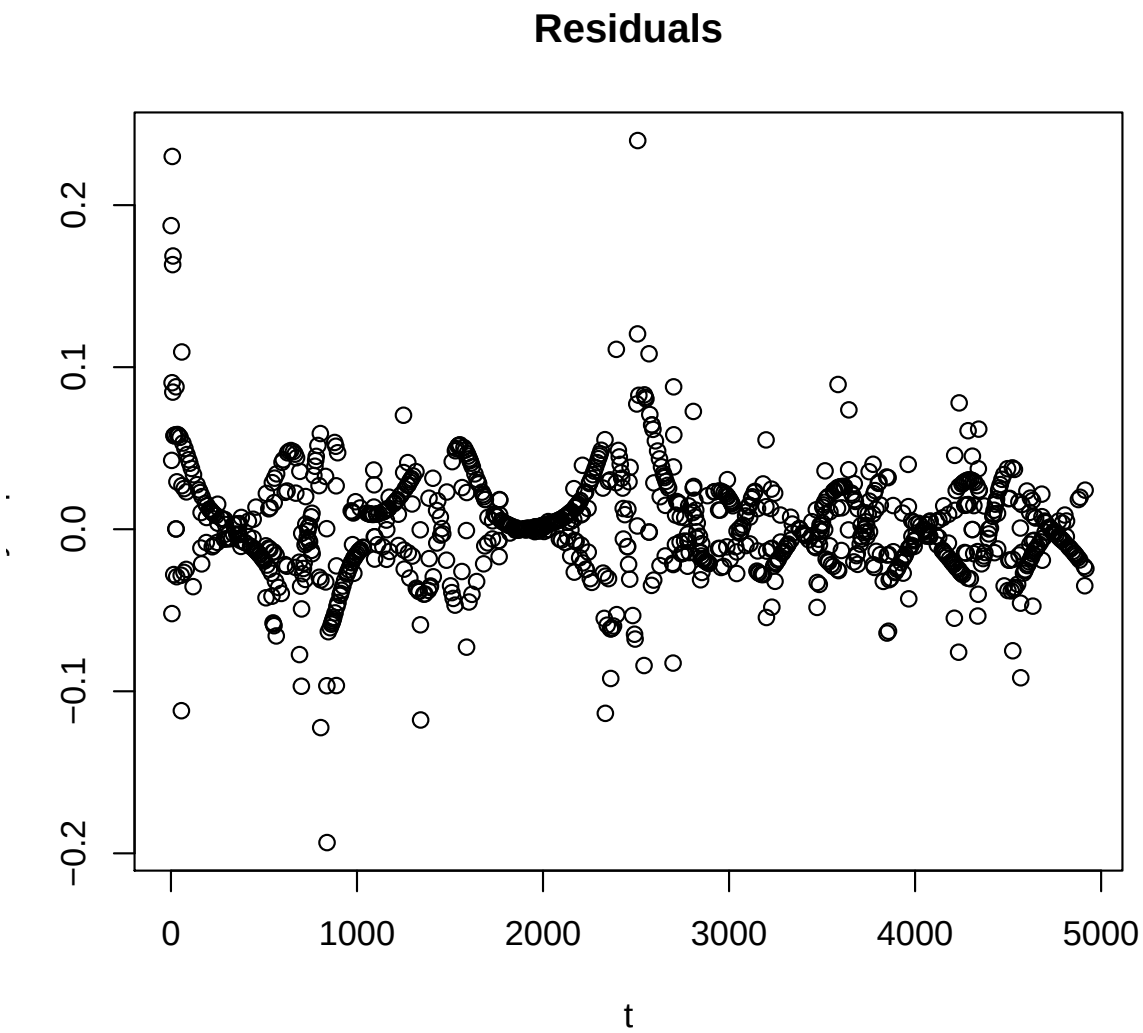
`R` is weak and refuses to do really big distance matrices

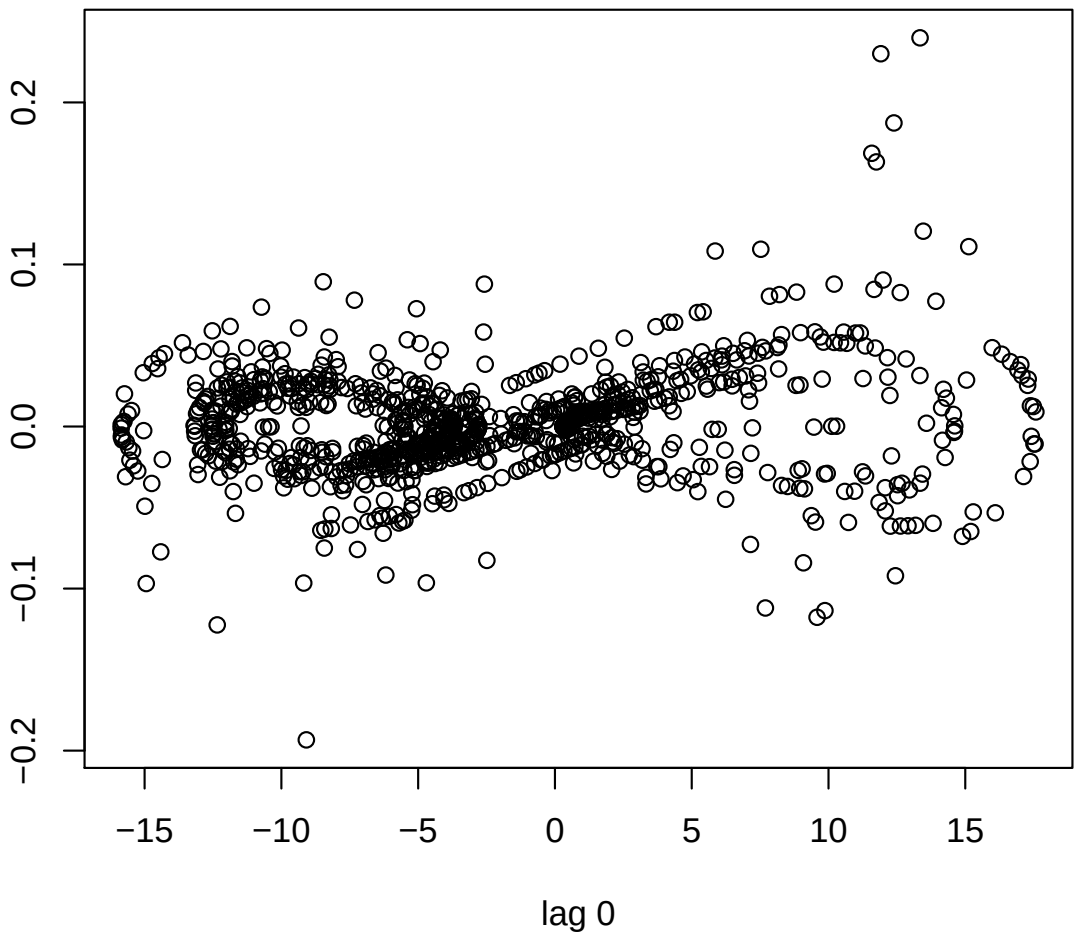
```
> lorenz.rcon = embedd(x.ts[1:5000],3,40)
> nrow(lorenz.rcon)
[1] 4920
> lorenz.dist = knn.dist(lorenz.rcon)
> lorenz.futures = x.ts[2:5001]
> train = sample(1:nrow(lorenz.rcon),0.8*nrow(lorenz.rcon))
> test = (1:nrow(lorenz.rcon))[-train]
> preds = knn.predict(train,test,lorenz.futures,lorenz.dist,
                      k=3,agg.meth="mean")
> plot(test,preds,col="red",xlab="t",ylab="x",type="p",
       main="3NN prediction vs. reality")
> lines(test,lorenz.futures[test])
> plot(test,lorenz.futures[test] - preds,xlab="t",
       ylab="reality - prediction",main="Residuals")
```


3NN prediction vs. reality
15
10
5
0
−5
−10
−15
0
1000
2000
3000
4000
5000
t

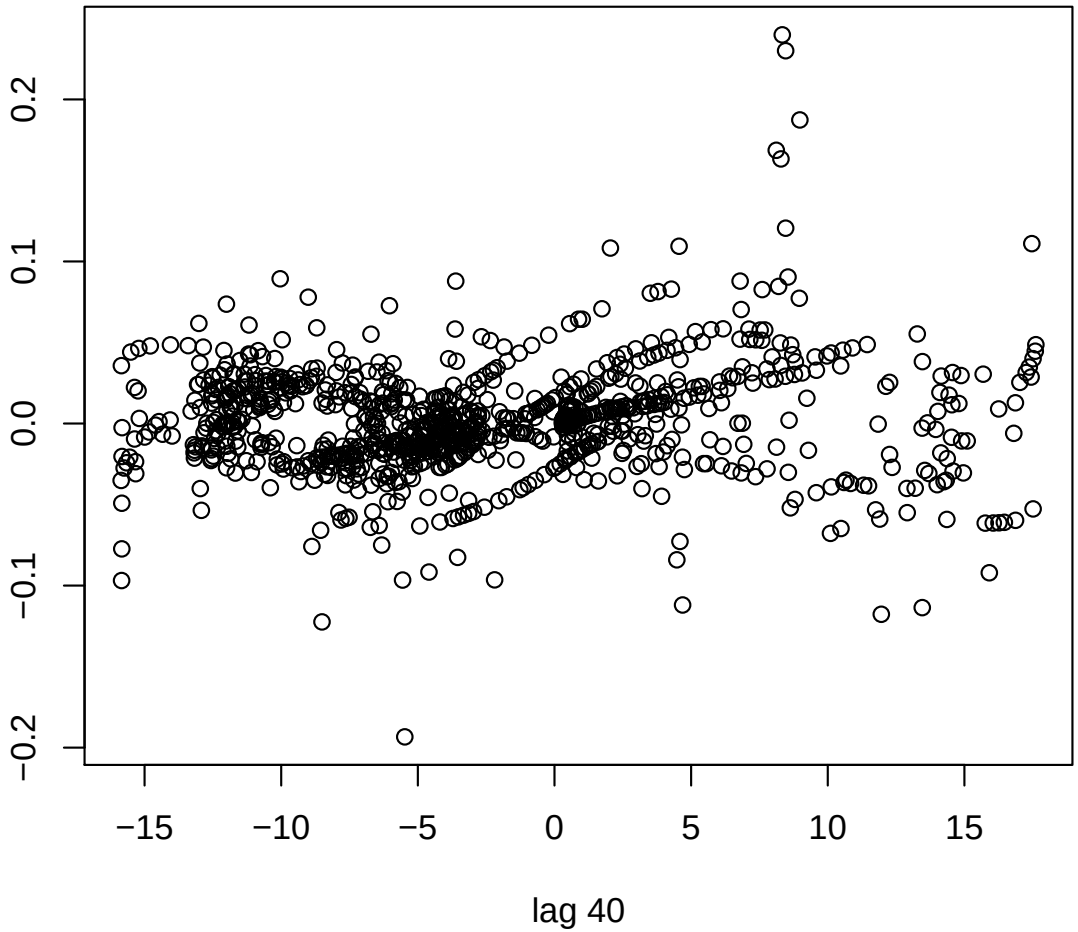

3NN prediction vs. reality
15
10
5
0
−5
−10
−15
0
1000
2000
3000
4000
5000
t

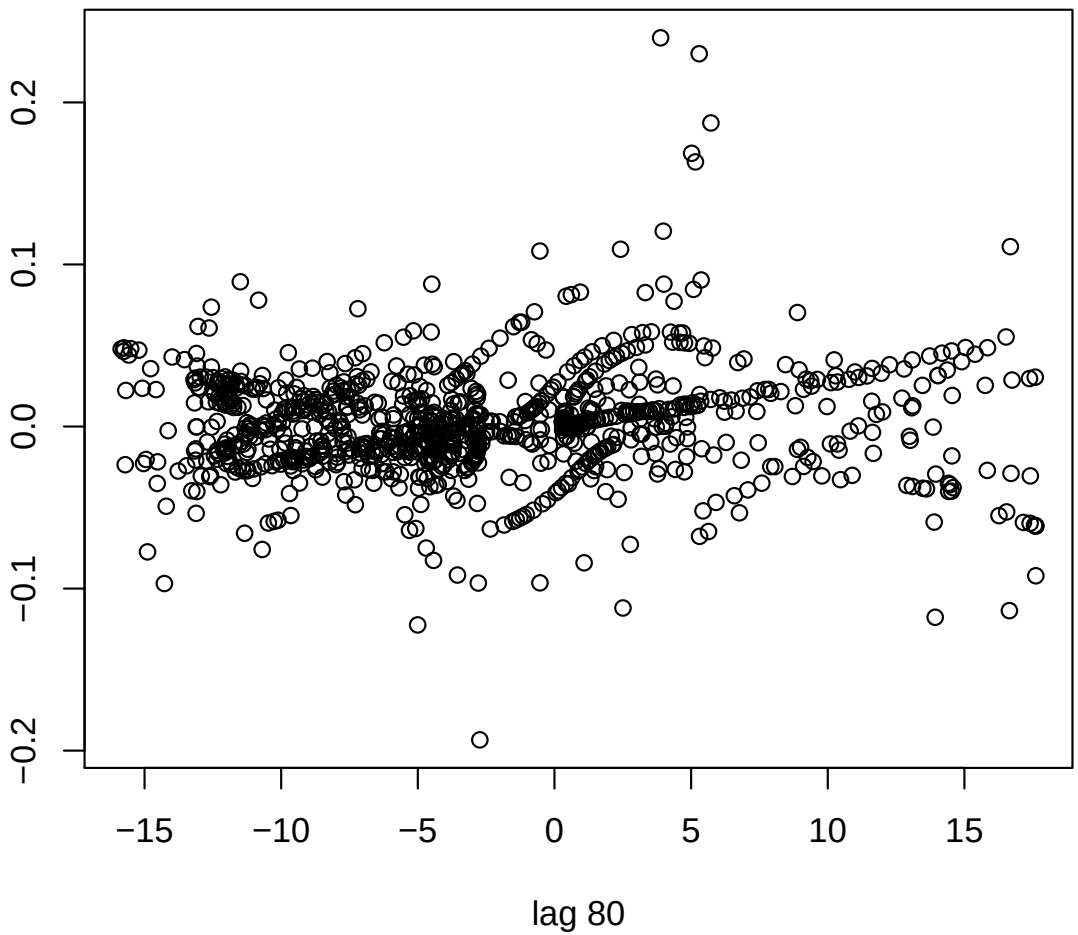
Not just a programming error!




Residuals vs. first history component
0.2
0.1
0.0
−0.1
−0.2
−15
−10
−5
0
5
10
15
lag 0

Residuals vs. second history component




Residuals vs. third history component
0.2
0.1
0.0
−0.1
−0.2
−15
−10
−5
0
5
10
15
lag 80

Why not just use huge k?
bias/variance trade-off

- small k: tracks local behavior, big change in prediction depending on which point just happens to be closest to you
- big k: smooth predictions over state space, less sensitive to sampling, less informative locally
- $k = n$: same prediction all over state space!

Can we somehow increase k with n, to take advantage of filling-in along the attractor? — See handout on kernel prediction.

Cross-Validation

Standard and useful way of selecting control settings

Principle: we don't just want to fit old data, we want to predict new data

i.e., don't just optimize **in-sample** error, optimize **out-of-sample** error

Problem: we don't know the distribution of future data!

Would we be trying to *learn* a predictor if we did?

Observation: we do have a sample from that distribution — our sample

$\Leftarrow$ ergodicity: long trajectories are representative

Solution: fake getting a new sample by sub-dividing our existing one *at random*

Chose the settings which generalize best, which can **cross-validate**

Random division into training and testing sets needs to respect the structure of the data

e.g. divide points in the embedding space, not observations from the original time series

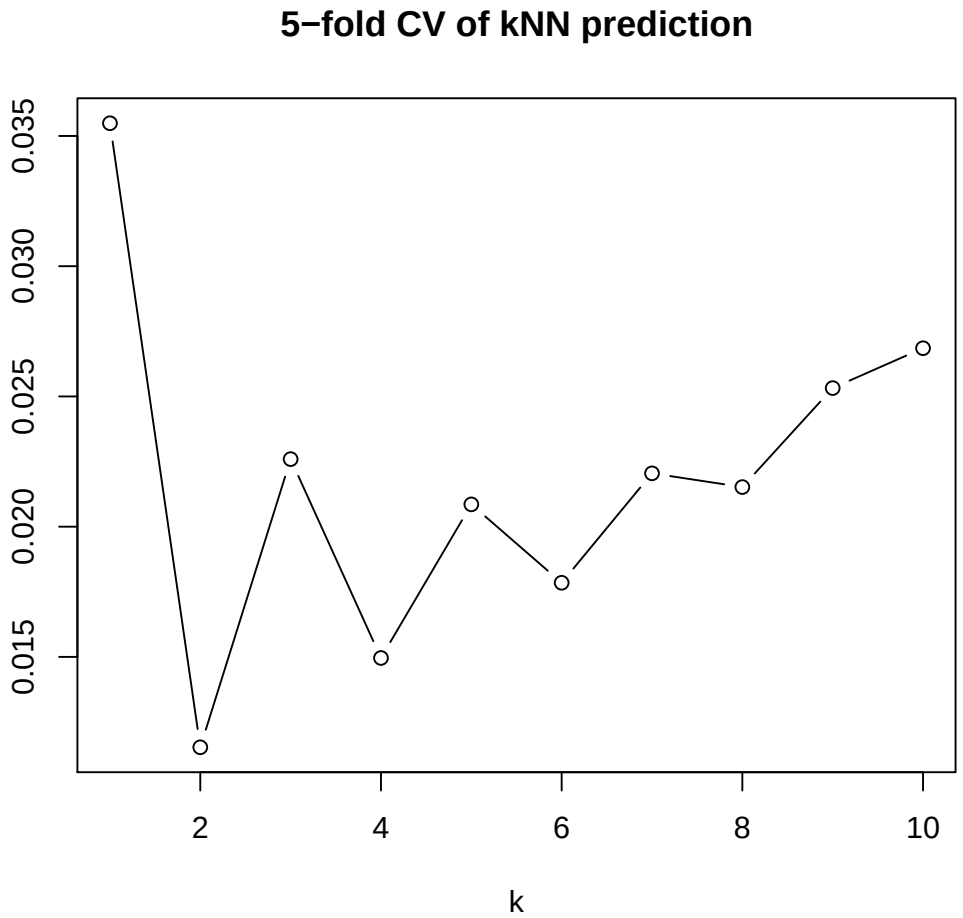
note: did this already with the Lorenz example — that was an out-of-sample prediction

Good idea to use a couple of random divisions and average out-of-sample errors

This **multi-fold** cross-validation also gives you an idea of the uncertainty due to sampling noise

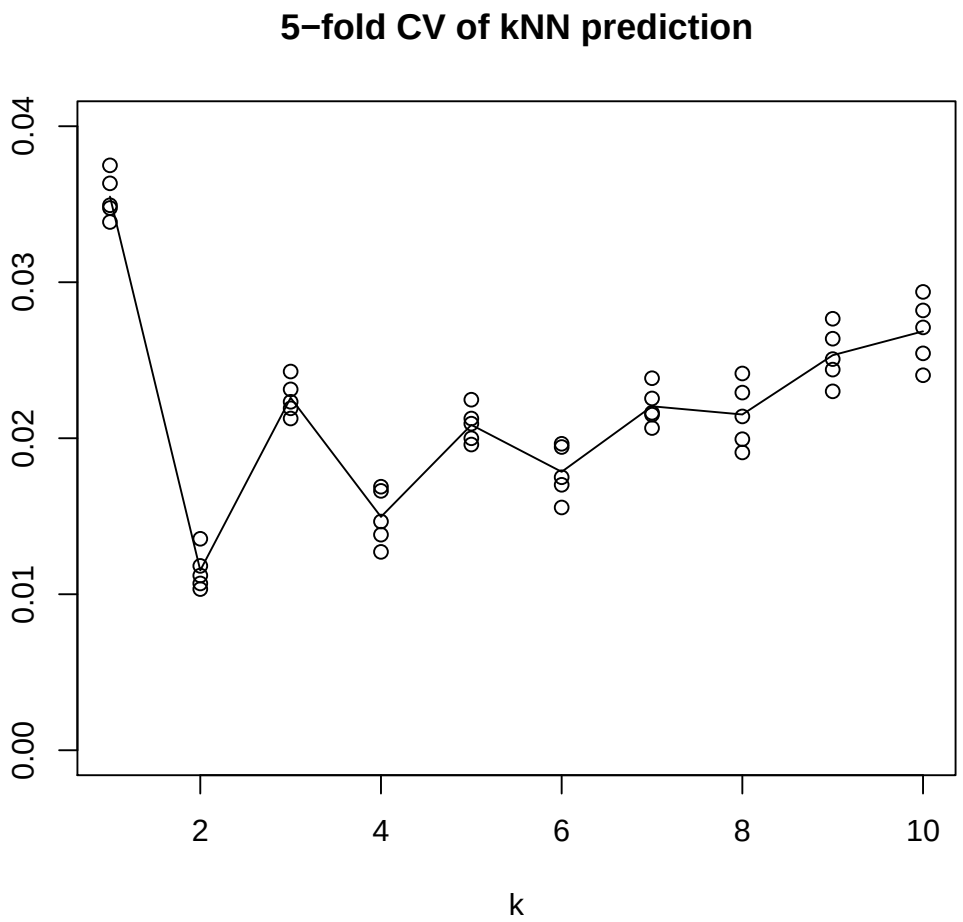
5-fold cross-validation of kNN prediction of Lorenz, $k \in 1{:}10$ Warning: slow!

```
fold = sample(1:5,nrow(lorenz.rcon),replace=TRUE)
cvpred = matrix(NA,nrow=nrow(lorenz.rcon),ncol=10)
cvprederror = matrix(NA,nrow=nrow(lorenz.rcon),ncol=10)
for (k in 1:10) {
  for (i in 1:5) {
    train=which(fold!=i)
    test=which(fold==i)
    cvpred[test,k] = knn.predict(train=train,test=test,
                                 lorenz.futures,lorenz.dist,
                                 k=k,agg.meth="mean")
    cvprederror[test,k] = lorenz.futures[test]-cvpred[test,k]
  }
}
mean.cv.errors = apply(abs(cvprederror),2,mean)
plot(mean.cv.errors,xlab="k",ylab="mean absolute prediction
     error", main="5-fold CV of kNN prediction",type="b")
```


5−fold CV of kNN prediction
0.015
0.020
0.025
0.030
0.035
2
4
6
8
10
k

Add the individual “fold” values to the previous plot graphics hygiene: have vertical scale run to zero

```
plot(mean.cv.errors,xlab="k",ylab="mean absolute prediction
     error", main="5-fold CV of kNN prediction",type="l",
     ylim=c(0,0.04))
error.by.fold = matrix(NA,nrow=5,ncol=10)
for (i in 1:5) {
  for (k in 1:10) {
    test=which(fold==i)
    error.by.fold[i,k] = mean(abs(cvprederror[test,k]))
    points(k,error.by.fold[i,k])
  }
}
```



Conclusion: 2 is best, but they're all pretty good
note bigger scatter at bigger k

Norman H. Packard, James P. Crutchfield, J. Doyne Farmer, and Robert S. Shaw. Geometry from a time series. *Physical Review Letters*, 45:712–716, 1980.

Floris Takens. Detecting strange attractors in fluid turbulence. In D. A. Rand and L. S. Young, editors, *Symposium on Dynamical Systems and Turbulence*, pages 366–381, Berlin, 1981. Springer-Verlag.