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Article

Bayesian Smoothing Splines

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Abstract: Fitting parameters on spline curves produces more parsimonious models, maintaining fit quality. Smoothing the splines reduces predictive variance. Individual splines are often fit by type of variable, e.g., in age-period-cohort models. Linear and cubic splines are most common. Several smoothing criteria have been used for parameter curves, with cubic splines fit by constraining the integral of splines' squared-second derivatives popular recently. Constraining the sum of squared second differences for linear splines is analogous. Generally the degree of smoothing is selected using cross-validation. Known spline dummy-variable matrices allow regression estimation of splines, with smoothing done via constrained regression. Smoothing criteria based on sums of squares or absolute values of parameters, as in ridge regression or LASSO, improves predictive accuracy and produces splines similar to smoothing by second-derivative constraints. Variables with very low t-statistics represent points where curve-shapes barely change. Eliminating those variables leaves knots concentrated where spline shapes change. A Bayesian version of this puts shrinkage priors on spline parameters. This yields realistic joint parameter distributions, avoids problems associated with using cross-validation for parameter estimation, and readily expands to non-linear modeling, such as interactions among variable types. Regularized regression and Bayesian spline methods are compared for two example datasets.

Keywords: smoothing splines; shrinkage priors; MCMC; Bayesian methods

1. Introduction

Complex trends in data can be represented with curves pieced together across the data. Linear splines consist of line segments that join up at the points. Cubic splines use adjoining segments that agree in their first two derivatives, so are smoother, and tend to give more realistic interpolations near the joints (knots). Design matrices have been worked out to create these splines by regression.

Splines can also be fit across sets of enumerated variables in more general models. For instance, APC (age-period-cohort) models could have splines for each of the three sets of variables. The three spline design matrices would combine into one for the whole model. This can produce more parsimonious models. Variables are need for each A, P, and C, but if adjacent parameters are similar, or lie on the existing curve, those spline parameters can be set to zero, as there is no change in the curve shape at those points.

Smoothing splines further increases model parsimony. Then the curves, and so the level parameters on the curves, do not swing as widely. This is a form of parameter shrinkage. Measures of curve smoothness are added to the negative loglikelihood (NLL), and are shrunk along with it . Before smoothing, the splines produce the same level parameters as would usual dummy matrices. Smoothing can improve predictive accuracy, although not fitting every value as closely. Here parameter-shrinkage methods like ridge regression, which are known to improve predictive accuracy, are investigated as smoothing

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criteria. Bayesian shrinkage using shrinkage priors is tried as well. This gives a wider range of smoothing choices.

Ridge regression, LASSO, and traditional spline smoothing cannot use likelihood penalized by parameter counts to compare models because shrunk parameters use up fewer degrees of freedom. Cross validation (CV) is used instead. The dataset is divided into a number of subsets, the NLL on each is calculated with the parameters estimated from the remaining data, and their sum is the CV NLL. It is thus an alternative method of penalizing the likelihood, and the degree of smoothing that optimizes the CV NLL is chosen. Estimating parameters by penalized likelihood has issues, however. The penalty is itself an estimate of sample bias – the overstatement of the likelihood due to measuring it on the sample used for fitting. The best penalized likelihood risks being the one with the greatest under-estimation of sample bias. From a Bayesian perspective, CV estimates are often close to the posterior mode. The Bayesian posterior mean of the shrinkage parameter comes from Bayesian shrinkage, and usually the mean is a better estimator than the mode, at least with regard to the estimation variance.

In a frequentist framework, parameters are constants that do not have distributions. But frequentists can use random effects, which are a lot like parameters with distributions. Their distributions are postulated, not subjective. But the same holds for priors in contemporary Bayesian analysis. They can be tested by model results just like other postulated distributions, like that of the data given the parameters. The main Bayesian engine is MCMC (Markov chain Monte Carlo) estimation, which samples from the joint likelihood of the parameters and the data. By the definition of conditional distribution this is the conditional distribution of the parameters given the data times the probability of the data. The latter is an unknown constant, and MCMC can sample without knowing it. In frequentist terms, it gives a sample of the conditional distribution of the random effects given the data. Being able to do this is largely a philosophical question for frequentists to decide. Some specifics are in the examples.

[1] give regression basis functions for cubic splines, with a derivation posted at [2]. Simplifying it a little, assume the spline has knots at the points *1:K*. They assume the spline is linear in [1,2] and [*K–1, K*]. Dummy variables a_j are defined for *j = 1:K*. For an observation from any real $z \in [1, K]$ they set $a_1(z) = 1$ and $a_2(z) = z$. Then for *j > 2* it works out that:

$$z > K - 1\text{: } a_j(z) = {(z + 2 - j)^3}\Big/{K + 2 - j} - (z + 1 - K)^3$$

$$z \le K - 1\text{: } a_j(z) = {(z + 2 - j)_+^3}\Big/{K + 2 - j}$$

[3] introduced a smoothing criterion for splines in general a century ago. The curve is differenced three times at each knot, and the sum of the third difference constrained. The integral of the squared second derivative of the curve gives a measure of its smoothness and is a popular criterion lately. With parameters β_j the value of the cubic spline at any point is $\sum_j \beta_j a_j(z)$. The integral of the second derivative squared comes out to be $\left(\sum_j c_j \beta_j\right)^2$ for some values c_j. This is a weighted sum of all the cross products of the parameters. It generally increases simultaneously with $\sum \beta_j^2$ and with $\sum |\beta_j|$, so constraining either of those, as in ridge regression or LASSO, also constrains the squared second derivative, giving similar smoothing.

[4] provide a basis for linear splines. Again, $a_1(z) = 1$. For *j*, *z > 1*, $a_j(z) = (1 + z - j)_+$. This gives a design matrix for the second differences of the level parameters.

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Then constraining $\sum \beta_j^2$ constrains the sum of the squared second differences along the curve, analogously to the integral of the squared second derivatives of the cubic spline.

[5] introduced ridge regression, minimizing NLL $+ \lambda \sum \beta_j^2$. They showed that there is always some $\lambda > 0$ that gives a lower error variance than $\lambda = 0$, which is the MLE (maximum likelihood estimation) case. MLE gives the minimum variance unbiased estimate. Ridge regression biases the estimates, generally by shrinking them towards the overall mean. Thus it ties in to Stein's Theorem ([6]), which says that with 3 or more means being estimated, the error variance is reduced by some degree of shrinkage towards the overall mean. With spline design matrices smoothing the splines generally improves the fit. There remains the issue of how much to shrink.

LASSO (least absolute shrinkage and selection operator), from [7], popularized by [8] instead minimizes NLL $+ \lambda \sum |\beta_j|$. This is used more because it sets some parameters to exactly zero, thus taking them out of the model. That is the selection part. It still reduces the error variance by shrinkage towards the overall mean, verified for each model by cross validation for λ.

2. Materials and Methods

The first example looks at a sample of USA workers compensation benefit payments arranged by year of accident (rows = cohorts) by time to payment (columns = ages), as in Table 1. The years of payment (periods) are the upward sloping diagonals. The logs of the payments are fit by APC regression models.

Table 1. Workers compensation benefits paid by accident year and lag

129124	217397	118421	63984	39196	31450	19809	14556	8420	8507	7319	8937	10274	5383	5594
216427	325705	171013	92336	65834	41287	28358	22541	15742	16934	12498	17058	10786	7834	0
190698	207945	132229	74989	41989	32347	26640	21860	26870	17868	15149	15073	10549	0	0
117415	166555	95082	55577	40785	28737	16396	15102	12993	16123	10323	8979	0	0	0
133903	196230	110738	68289	52485	31817	23922	25356	17653	13431	14458	0	0	0	0
201997	289239	165234	103281	70280	57042	39964	34252	25683	21589	0	0	0	0	0
293284	435794	242665	159174	108122	75959	53191	42359	35453	0	0	0	0	0	0
409026	605225	381820	235599	162399	113710	81298	70265	0	0	0	0	0	0	0
514682	799168	437650	281391	203616	143531	109599	0	0	0	0	0	0	0	0
674265	886002	512631	364672	263383	215784	0	0	0	0	0	0	0	0	0
692986	905049	546113	396918	266963	0	0	0	0	0	0	0	0	0	0
700094	929014	590184	366655	0	0	0	0	0	0	0	0	0	0	0
627820	834302	517097	0	0	0	0	0	0	0	0	0	0	0	0
449942	552715	0	0	0	0	0	0	0	0	0	0	0	0	0
326810	0	0	0	0	0	0	0	0	0	0	0	0	0	0

The second example is log mortality rates for Danish women found in the Human Mortality Database for ages 50 – 89 for years of death 1967 – 2016. The mortality rates are computed as the number of deaths divided by the applicable population. The data used is age by year, with cohort computed as year of death – age at death. These year:age cohorts approximate the year-of-birth cohorts. With 50 ages and 40 periods there are 40 + 50 -1 = 89 cohorts, 1878 – 1966. The variables for each direction are numbered consecutively 1, 2, 3… .

The linear and cubic spline design matrices are built for each dataset. The logs of payments and of the mortality rates are put into column vectors, with parallel vectors used to track the age, period, and cohort of each observation. The first age, period, and

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cohort are left out for the linear splines, with a constant term included as a column of all 1's. The three individual-dimension spline design matrices are combined into larger ones for the datasets, with the age, period, and cohort variables grouped in columns.

These combined design matrices are singular because of the overlap among the three directions. There is no apparent way to eliminate the overlap and get true effects for each direction. Even leaving out a direction does not help. Fitting an age-period model with no cohorts implicitly assumes that there are no cohort effects, and the parameters are those for this assumption. It is testable by reviewing residuals by cohort. For spline models, some variables will naturally be eliminated – those for ages, periods, and cohorts where the curve shape changes minimally. Leaving out such variables makes the design matrix invertible. In the first example, the age-cohort model was fit first, and the least-significant variables were taken out, and then the period variables were put in. For the second example, the cohorts were left out initially.

The variables to eliminate were identified by a LASSO fit on the spline design matrices, using the R package glmnet. The function cv.glmnet does a cross-validation exercise for λ, using their algorithms to find a range of values for λ. One output is $lambda.min, which they identify as the smallest reasonable degree of shrinkage. The variables whose parameters it sets to zero were the ones eliminated. This was done again once the third direction was put back in, leaving a starting set of variables for the analysis. Some of those latter also went to zero. For the cubic splines, the first variable in each direction is the constant term. Only one of those is kept. The second variable gives the age, period, or cohort number for the direction. Because cohort = period – age, these variables are linearly dependent, and one must be left out. In these examples, that already happened at the first LASSO stage. Also, glmnet adds a constant that is not shrunk, so the constant term is left out of the design matrix for this step.

Ridge regression parameter estimates for a given λ have a closed-form expression that simplifies cross validation and Bayesian analysis. With design matrix x and data y, straight regression parameters are given by:

$$\beta = (x'x)^{-1}x'y$$

With U parameters, let J be the UxU identity matrix with the upper right element replaced by zero. Then the ridge-regression estimate is:

$$\beta = (x'x + \lambda J)^{-1}x'y$$

The sum of squared residuals is $\sum(y - x\beta)^2$. This computes quickly enough to easily do leave-one-out (loo) cross validation for λ, and this takes only a few lines of R code. Just loop through the observations, computing for each the squared residual, and so the log-likelihood, with the parameters fit without that observation. Standard R non-linear optimization software can quickly find the cross-validation λ with the highest loo loglikelihood. This is done for each example using cubic and linear splines.

The implementation of MCMC is done with the Stan system, using the Rstan and CmdStanR packages. The code is run from R but coded in the Stan language, which is converted to C++ and compiled. Mainly it takes in the data and has code for the prior distributions. Here the priors for the parameters β, but not the constant, were taken as mean-zero normals with parameter s. This is considered Bayesian ridge regression, as the NLL of the parameters is a constant $+\beta^2/2s^2$, so their sum is $\lambda\sum\beta_j^2$, $\lambda = 1/2s^2$. The residuals are postulated to be normal with standard deviation *sig*. Both log(s) and log(sig) are assumed to be uniform distributed in [–6, 6], and the constant is uniform on $\pm 1.8 \times 10^{308}$, which is the limit of double-precision numbers on most computers.

Bayesian LASSO puts double-exponential priors on the parameters. The NLL is then a constant$+ |\beta|/2s^2$, so gives LASSO. It does not, however, set any parameters identically

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to zero over the entire sample. It does for some parameters in most samples, but this can vary across the samples, so the means are never exactly zero.

The double exponential distribution is similar to a Students t-distribution with six degrees of freedom. With matching scale parameters, they agree in variance and kurtosis, and so in all existing positive moments of that t-distribution, in that the odd moments are zero for both. The different shapes close to zero are due to differing moments of 1/X for the positive half of the distributions. The normal is of course the limit of the t as the degrees of freedom increases, and for degrees of freedom less than six, the t gets more heavy-tailed. The case of two degrees of freedom is sometimes a good shrinkage prior. It has:

$$F(x) = 0.5 + 0.5x[2s^2 + x^2]^{-0.5}$$

$$f(x) = (2 + [x/s]^2)^{-1.5}/s$$

Then for each β, $-\log(f(\beta)) = 1.5\log(2 + [\beta/s]^2) + \log(s)$, so for a fixed s, the constrained estimation would minimize $\text{NLL} + \sum_j \log(2 + [\beta_j/s]^2)$. That would constrain larger parameters less than the sum of squares or absolute values does, so would allow greater relative deviation from zero for larger parameters. It also shrinks the smaller parameters more.

Intermediate between cross validation and fully Bayesian estimation of λ is a hybrid constrained Bayesian estimation. This is Bayesian estimation of the loo cross-validation λ. It estimates λ using the full spline design matrix, where the fitted value for each point for a given λ is the ridge-regression fitted value excluding that point. The residuals are still taken to be normally distributed with standard deviation *sig*, which is the other parameter in the model. The β parameters are an intermediate calculation.

This can run much faster and generally gets mean β parameters close to those from the full Bayesian analysis, but with much lower standard deviations. It generates a distribution of λ, and often its mode is close to the cross-validation λ.

The full Bayesian estimation builds a sample distribution of all the parameter sets that could have generated the data. The hybrid method has just the parameter sets that are ridge-regression parameters from some λ. That would not be as useful for distributional projections from the model but would provide a look at the parameters and the distribution of λ.

Stan uses MCMC to create a sample of the conditional distribution of the parameters given the data. It also provides an estimate of the loo cross-validation loglikelihood for the whole sample using Pareto-smoothed importance sampling [9]. The entire distribution of *s* would be provided for risk analysis. A point estimate could be selected as the mean s from the conditional distribution. This avoids using cross-validation for parameter estimation. Also the cross-validation estimate of *s*, under some common assumptions, is more like the mode of the conditional distribution.

The distributions postulated for the β parameters are also in the typical setup for random effects, but in that case the constant, *s*, and *sig* are parameters. There is no apparent reason that these three could not also be taken as random effects with the postulated distributions. With that step, MCMC could be used in a frequentist estimation.

3. Results

Table 2 shows the resulting λs and loo cross-validation sum of squared residuals (SSR) for linear and cubic splines for the two examples.

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Table 2. Ridge-regression loo cross-validation results

	Example 1 Linear, Cubic		Example 2 Linear, Cubic	
λ	0.342	0.004	25.36	0.202
SSR	2.163	3.138	8.046	11.21

A higher λ for a given model means that more shrinkage was applied. The linear models smoothed more and had better fits by loo cross-validation SSR than did the cubic models.

The variables remaining for each model after LASSO with MCMC-fitted parameters are given in Table 3. The variables are identified as a, y, or c for age, year, or cohort. In the linear splines, the first age, year, and cohort are left out for identifiability, and this is also done for the cubic splines as those variables are all constant terms.

The hybrid MCMC – cross-validation estimated λ for Example 1, linear splines is 0.402, with a mode of 0.291. The cross-validation estimate of 0.342 is between these. The cubic-spline estimate is 0.0066, with mode of 0.0048, which is still higher than 0.0040 from cross-validation. The means are higher than the modes as is usual for positively skewed parameter distributions, and they were higher than the CV estimates. Calculating modes for sample distributions is a bit involved. The R modeest package was used here with the half-sample mode estimator. That finds the smallest interval with half the sample in it, then repeats for that half, etc.

For Example 2, the MCMC linear spline λ is 22.0 with standard deviation 7.7 and mode 24.4, compared to λ of 25.4 from cross validation. The mode is close to the CV estimate, but now the distribution seems to be negatively skewed. The MCMC cubic-spline λ is 0.0033, which gives less shrinkage than the λ = 0.2 from cross validation. The MCMC and hybrid estimations here followed some of the cohort variations in more detail than did cross validation – which had a better SSR than the hybrid did.

In both examples for both splines, the hybrid β parameters are close to those from the full MCMC, and the resulting level parameters on the splines are difficult to distinguish in a graph. Naturally, though, the parameter standard deviations from the hybrid fit are much smaller, as the parameters are constrained to be ridge-regression results.

The loo penalized loglikelihood for the linear spline fit in Example 1 is 74.9, with a standard error of 11.9. For the cubic spline it is 52.0 with a standard error of 8.5. They are about 2 standard errors apart, so the linear spline fit is probably but not definitively better.In Example 2, the linear spline loo is 2676 with a standard error of 39.3. The cubic loo is 2376.5 with standard error 42.2. The linear spline fit is somewhat better there as well.

There are splines fit to each of age, year, and cohort components for each example. The sum of these components plus the constant term gives the fitted value for a data point. Figure 1 graphs these six splines for the Workers Comp payment example, Example 1, for the MCMC fits. The other fits give splines that are visually indistinguishable from these. Even though the cross-validation estimation shrinks less, the splines are robust to small changes in λ. This makes the weakness of cross validation less important but of course MCMC gives better interval estimates.

In this example there are 15 intervals in each direction, so they work on one graph. The cubic splines are smoother. The linear splines show corners where the slope changes, but the parameter shrinkage keeps them reasonably smooth. The cubic and linear splines in each direction look like rotations of each other. These offset to give similar fitted values.

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Table 3. Variables left after LASSO with MCMC parameter estimates

Ex. 1 Linear		Ex. 1 Cubic		Ex.2 Cohort Linear		Ex.2 Cohort Cubic		Ex. 2 All Other	
cn	11.87	cn	11.47	c2	-0.0056	c3	-0.0033	Linear	
y2	0.289	y2	0.092	c3	-0.0060	c9	0.02559	cn	-5.1208
y4	-0.098	y6	0	c30	0.0028	c10	-0.0773	a2	0.0825
y6	0.074	y8	0	c31	0.0017	c11	-0.0199	a10	-0.0043
y8	0.036	y9	0	c32	0.0018	c12	0.14383	a11	0.0071
y9	0	y10	0.013	c33	-0.0028	c13	0.0283	a12	-0.0022
y10	0	y11	-0.025	c34	0.0004	c14	-0.0339	a19	0.0087
y11	0.061	y14	0.008	c35	0.0042	c15	-0.1202	a25	-0.0052
y14	-0.107			c36	0.0033	c16	-0.0177	a26	0.0181
y15	0.071			c37	0.0020	c17	0.08452	y30	-0.0063
c2	0.119	c2	0.415	c38	0.0034	c18	0.03676	y31	-0.0044
c3	-0.484	c3	-1.848	c50	-0.0015	c19	-0.0374	y34	-0.008
c4	-0.232	c4	3.163	c51	0.0026	c20	-0.0984		
c5	0.507	c6	-1.769	c52	-0.0003	c21	0.10715	Cubic	
c6	0.159	c7	0	c53	0.0029	c24	-0.0175	cn	-5.16
c9	-0.157	c8	0.425	c54	-0.0026	c40	0.08974	a3	0.1285
c10	-0.025	c11	0	c55	-0.0069	c41	-0.1814	a7	-1.4956
c11	-0.192	c12	0.012	c56	-0.0220	c42	-0.0154	a8	2.2623
c12	-0.032			c63	0.0004	c43	0.25192	a9	-0.5971
c13	-0.113			c64	0.0120	c44	-0.2621	a10	-0.7382
c14	-0.168			c65	0.0073	c45	0.09924	a11	0.5747
a3	-0.785	a3	-0.748	c66	0.0019	c46	0.24626	a12	-0.1344
a5	0.105	a5	2.904	c67	-0.0031	c47	-0.1843	y3	-0.0002
a6	0.023	a6	-3.018	c68	-0.0053	c48	-0.4701		
a8	0.13	a7	0.916	c69	0.0023	c49	0.65241		
a10	0.061	a10	-0.071			c50	-0.2266		
a12	0.143								
a13	-0.188								
a14	-0.029								

The cubic splines are graphed with dots at intervals of 0.2 to show the smoothness of interpolation. They were fit at intervals of 1.0, or possibly even longer if some parameters went to zero. The jumps in the last interval are a bit misleading. The basis functions were set up to make the splines linear within the first and last intervals with the same slope, given by the coefficient of the second spline variable. That's what looks like a jump near the right side of the graphs. But only the ending point of the interval was used in the fitting. Visually those final points appear to continue the curves established in the prior intervals. It would probably not be difficult to devise a new spline basis that just continues the current spline without making it linear in the last interval.

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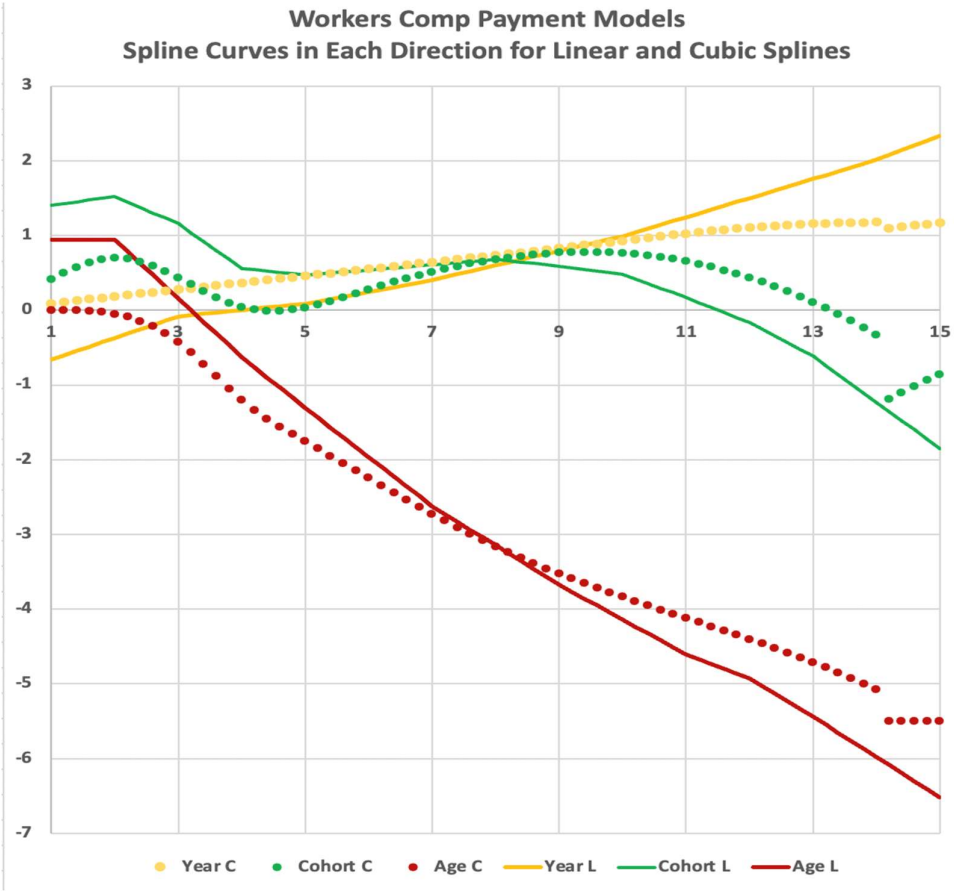

Figure 1. Spline curves Example 1, denoted as C or L for cubic or linear

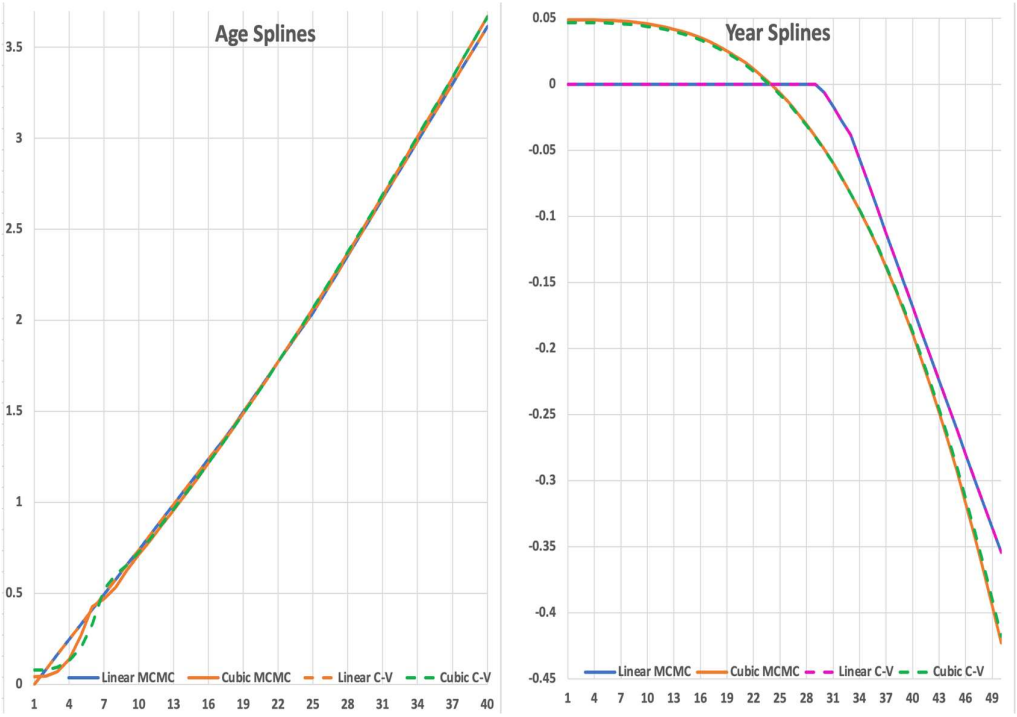

Figure 2. Age and year spline curves Example 2, denoted as MCMC or C-V.

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For Example 2, Danish female mortality, there are different numbers of points in each direction so separate graphs are used. Also the MCMC and cross-validation curves are slightly different, especially for cohort variabless for cubic splines. Figure 2 graphs the age and year splines and Figure 3 shows the cohort curves.

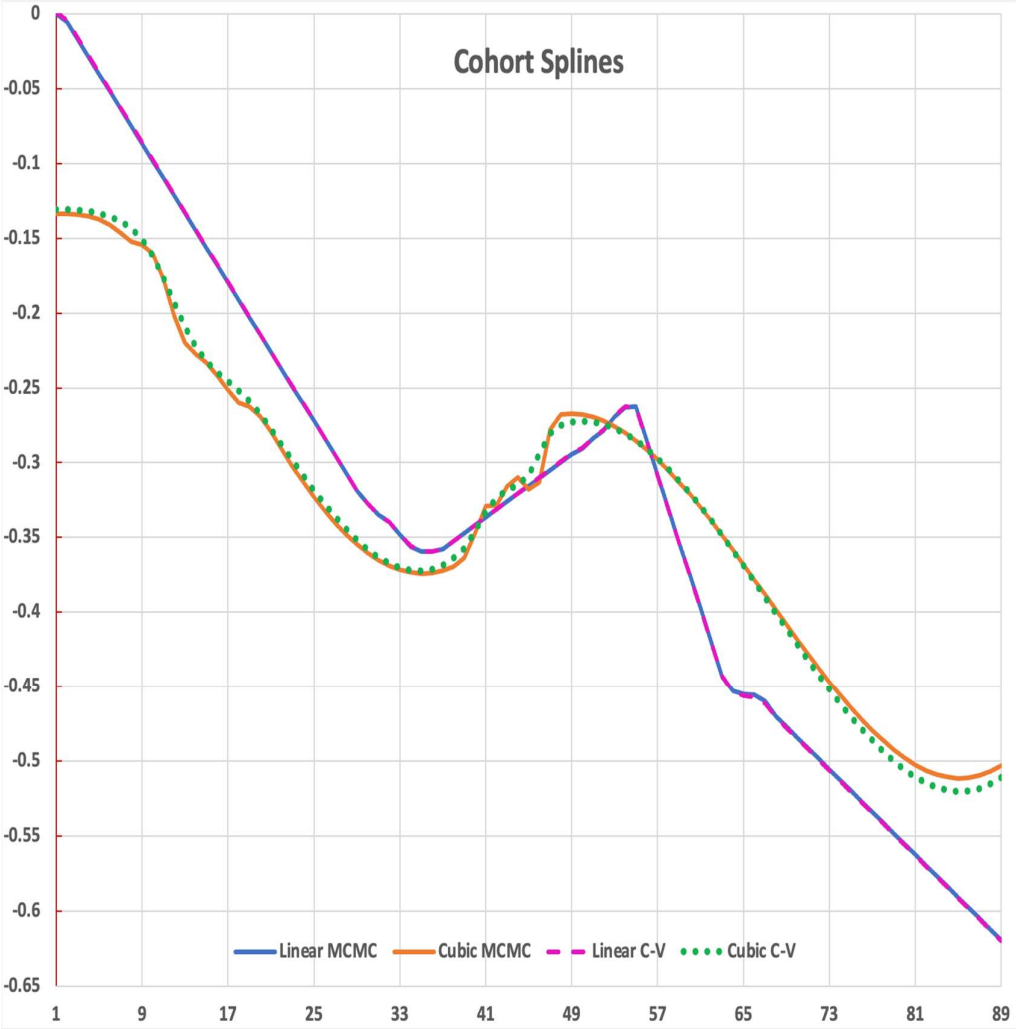

Figure 3. Cohort spline curves Example 2, denoted as MCMC or C-V for cross validation.

The cross-validation and MCMC linear splines again look the same, and the cubic splines are smoother, but with more twists and turns. The cubic spline fit by MCMC was shrunk less and shows more detailed movements than the one fit by cross validation, especially for the cohort splines. The cross-validation cohort spline, where those details were smoothed over, was better.

In the linear spline fit, the cohort trend overall was almost double the time trend. This included a sharp increase starting for cohorts born in 1912, peaking around 1932, and not getting back to the previous trend until those born in the early 1940s. This is not a typical pattern. [9] and [10] studied Danish mortality drivers and found that smoking behavior is a cohort effect that explains much of the historical mortality pattern. Smoking tends to be a life-long habit, so would be a cohort effect. They found that there had been a strong increase in smoking among Danish women born between the two world wars, which is consistent with the model results here.

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4. Discussion

Using parameter shrinkage for spline smoothing results in reasonably smooth splines, and shrinkage methodology has known advantages, like reduction in error variances. LASSO software can be applied directly, and minimal LASSO shrinkage usually eliminates a few variables, and with them those knots, where the curve shape does not change much. The knots end up concentrated in areas where the shape changes the most.

Ridge-regression smoothing for a given λ can be fit quickly with a single numeric calculation. This makes it fast and easy to use cross-validation for estimation of the smoothing constant λ. Bayesian shrinkage priors in MCMC give full distributions of the parameters and the resulting spline curves, and of λ as well. They also avoid problems with cross-validation parameter estimation like understating sample bias and estimating by the mode. The overall fits to the data are not particularly sensitive to the degree of shrinkage, however, which mitigates the CV problems.

Linear splines had largely been abandoned for being too jagged, but spline smoothing helps with that. In these examples, the cubic spline curves are smoother, but the linear splines are not too jagged and give better fits. They may have more flexibility in matching the changes in curve shapes needed here. A hybrid using MCMC in cross validation averts some problems with CV estimation, and is faster than straight MCMC, but does not produce the full distribution of possible parameter sets. For one of the cubic splines, CV seems to give a more useful model than do the hybrid or Bayesian approaches.

Having simple formulas for spline smoothing enables modelers to put smoothing spline fitting into their own code for model development. MCMC does not require linear models, and spline parameter shrinkage can be included as needed in a wide variety of models. Some nonlinear extensions of Example 1 using linear splines are briefly covered next as illustration.

It is common to start with a model for logs of the data, and then use a log link for fitting to the original unlogged values. Fitting a gamma distribution with a log link is widely used in General Linear Models (GLM). The j^{th} observation is postulated to be gamma distributed in a_j, b_j, which has mean and variance $a_j b_j, a_j b_j^2$. Usually some simplifying relationship among these parameters across the observations is assumed. In GLM the assumption is $a_j = a$, so this parameter is constant across the observations. Then the log link can give the b_j parameters. The gamma's mean squared divided by its variance is a, so is then constant for all observations. Thus the variance is proportional to the square of the mean. But if b is taken to be constant across the observations, then it gives the variance divided by the mean, which then is constant. In general, you could get the b_j parameters from the log link and then for an estimated constant c, and any power p you want, make the variance $= c\mu^p$ by setting:

$$a_j = \left(c b_j^{p-2}\right)^{1/(1-p)}$$

Then:

$$c\left(a_j b_j\right)^p = \left(c b_j^{-p}\right)^{1/(1-p)} = a_j b_j^2$$

Another popular generalization is to include interactions among the directions in the model. In mortality this started with the model of [11] that has the period trend modified by age. This is reasonable as medical improvements, etc., affect some ages more than others. Later [12] added cohorts to this model. The mean log mortality rate in year i for age j is:

$$m_{ij} = cn + a_j + y_i^{b_j} + c_{i-j}$$

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This was used with linear splines in MCMC with a negative binomial fit and a log link by [13] and [14]. Like the gamma, there are two forms of the negative binomial that can be used, although GLM only uses one of them.

The model of [12] also works for Example 1. The period trends in workers compensation in the US are driven by medical cost inflation. The payments include wage replacement as well but that is usually not inflation adjusted. The wage portion also caps out in a few years for most workers. Medical becomes a growing part for later claim ages (which are the payment times since injury), and so the period trend affects later payments more.

The MCMC loo cross-validation loglikelihood is 74.9 for the APC log model above. This improves to 85.9 by including these interaction effects. Assuming a lognormal distribution for the actual losses using the log link produces all the same parameters but with a loo of –1266.6. Likelihoods are lower for the unlogged values as the numbers are more spread out and the density is lower. For the gamma distribution with variance proportional to mean-squared, as in GLM, the loo is slightly worse, at –1268.3. With variance proportional to mean, it is better, at –1257.7. Finally, using the t-distribution with two degrees of freedom as the shrinkage prior brings this up to –1244.1, with a standard deviation of 13.6. Each step gives a possibly better result, and they add up to a meaningful improvement. The interaction term, choice of gamma distribution, and t-2 shrinkage prior are examples of the nonlinear modeling methods that can be built with spline models.

One limitation of Stan is that there are some probability distributions it cannot handle, including the Tweedie and the Poisson-Inverse Gaussian, which is a heavier-tailed negative binomial. These have good R apps but those are specialized and Stan hasn't included them yet. The Poisson-Inverse Gaussian uses modified Bessel functions which move very slowly. It can take 40-50 digits of accuracy to compute their changes, and double-precision computers need special software for that. Stan cannot just call the R apps because it converts to C++ and compiles. There are MCMC packages that can call anything from R, but right now they are significantly slower.

The discussion here has emphasized what Bayesian shrinkage can do for smoothing splines, but the flip side of that is what smoothing splines can do for Bayesian shrinkage. Nearby parameters that are similar, or change in a regular way, can be put on splines that use fewer parameters. That can increase the parsimony and predictive accuracy of shrinkage models. Also it can help address the overlap problem of APC modeling. In APC models it is not always possible to eliminate variables with low t-statistics, as variables are needed in every position. Splines can deal with that in that omitted variables are just points where the curve shape doesn't change. The two methodologies work well in combination.

Data Availability Statement: The Danish mortality data is from the Human Mortality Database, University of California, Berkeley (USA), Max Planck Institute for Demographic Research (Germany) and United Nations, https://www.mortality.org/. For Danish data, go to the country section of https://www.mortality.org/cgi-bin/hmd/hmd_download.php. Download the zip file (free account needed) and then find Exposures_lexis.txt and Deaths_lexis.txt under STATS.

Conflicts of Interest: The author declares no conflict of interest.

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Appendix A

This appendix has selected R and Stan code used in the study. This one is for LASSO.

```
library(glmnet)  # Lasso app
library(readxl) # Allows reading Excel filees
y=scan('logLoss.txt')  # reads in txt file as vector
xl = as.matrix(read_excel('lin_spline_dummy.xlsx')) # use either one of these
xc = as.matrix(read_excel('cub_spline_dummy.xlsx')) # For lasso leave constant out of design matrix

lin_fit = cv.glmnet(xl,y,standardize = FALSE)
lin_fit$lambda.min #lminimal lambda from cross validation
out = coef(lin_fit, s = "lambda.min")
out= as.matrix(out)
write.csv(out, file="out_lin.csv")
out
```

Now the R function for cross validation with ridge regression.

```
y1=scan('comp_log_y.txt') #then design matrices with constant term
xl = as.matrix(read_excel("comp_lin_lasso.xlsx"))
xc = as.matrix(read_excel("comp_cub_lasso.xlsx"))
x1 = xc # note x1 is with number 1, not l
n = ncol(x1)
m = nrow(x1)
Il = diag(n)
```

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```
Il[1,1] = 0
# define function to calculate loo for given lambda
loo_sse <- function(lam){
  loo = 0
  J = lam*Il #Il is n x n identity matrix with Il[1,1]=0
  for (j in 1:m){
    x = x1[-j,] # x1 and y1 have all rows
    y = y1[-j] # Negative indexes in R leave out the row or column
    beta = solve(t(x)%*%x + J)%*%(t(x)%*%y)
    loo = loo + (y1[j] - x1[j,]%*%beta)^2
  }
  return(loo)
}
ridge = as.numeric(optimize(loo_sse, lower = 0, upper = 30))
lambda =  ridge[1]
ridge
lambda # minimum solved for
beta = solve(t(x1)%*%x1 + lambda*Il)%*%(t(x1)%*%y1)
beta #parameters at minimum lambda
```

This is the R code to set up the Stan run for the hybrid CV-MCMC fit. It uses design matrices that include the constant term.

```
library("loo")
library(rstan)
rstan_options(auto_write = TRUE)
options(mc.cores = parallel::detectCores())
# last two  lines are some recommended Stan options
dmat = as.matrix(read_excel('lin_spline_dummy_cn.xlsx'))
dmat = as.matrix(read_excel('cub_spline_dummy_cn.xlsx'))
y = scan('logLoss.txt')
N <- nrow(dmat)
U <- ncol(dmat)
c(N,U)
xpx = array(0,dim = c(N, U, U))  #in R make 3D array of x'x missing one data point
for (i in (1:N)) {xpx[i,,] = t(dmat[-i,]) %*% dmat[-i,]}
xpy = array(0,dim = c(N,U))  # 2D array of x'y
for (i in (1:N)) {xpy[i,] = t(dmat[-i,]) %*%y[-i]}
Iminus = diag(U)
Iminus[1,1] = 0
df = list(N=N,U=U,dmat=dmat,y=y,xpx=xpx,xpy=xpy, Iminus=Iminus)
#now run stan with the arrays fed to it
set.seed(4)
```

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```
fit_2 <- stan(file = 'lam_ridge_mcmc.stan', data=df, verbose = FALSE, chains = 2, iter = 30000, warmup = 50
00, control = list(adapt_delta = 0.9, max_treedepth = 18))
```

This is the Stan code it calls – `'lam_ridge_mcmc.stan'`.

```
data {
  int N;          //number of observations
  int U;          //number of variables
  matrix[N,U] dmat;  //design matrix with U columns
  vector[N] y;     //the triangle in a column
  matrix[U,U] xpx[N];  //acts like a vector[N] of UxU matrices xpx
  vector[U] xpy[N];  //acts like a vector[N] of U vectors xpy
  matrix[U,U] Iminus;  //Identity matrix with 1,1 element = 0
}
parameters {  // both get uniform prior on defined ranges, the default
 real<lower=0, upper = 1> sig;
 real<lower=0, upper = 35> lam;
}
transformed parameters {
 vector[N] yhat; //fitted values of each observation when it is left out
 vector[N] yyhat; //fitted values using all points
 vector[U] beta;  //parameters from lambda using all points
 beta  = ((dmat'*dmat)+lam*Iminus)\(dmat'*y); //In Stan, matrix multiplication is *
 yyhat = dmat*beta; //not used but these fitted values are in output files
 for (j in 1:N) yhat[j] = dmat[j,]*((xpx[j] + lam*Iminus)\xpy[j]);
} //here xpx[j] is xpx leaving out the j observation; xpy similar
model { //fitting y using the left-out regression estimates
for (j in 1:N) y[j] ~ normal(yhat[j], sig);
}
generated quantities { //outputs log likelihood for looic
  vector[N] log_lik;
for (j in 1:N) log_lik[j] = normal_lpdf(y[j] | yyhat[j],sig);
}
```

The straight MCMC run uses the design matrix without the constant term and calls the Stan code.

```
x = dmat
n = N
u = U
df = list(n=n,u=u,x=x,y=y)
set.seed(4)
fit_3 <- stan(file = 'beta_ridge.stan', data=df, verbose = FALSE, chains = 2, iter = 2000, warmup = 1000, c
ontrol = list(adapt_delta = 0.84, max_treedepth = 20))
```

This is `'beta_ridge.stan'` that it calls.

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```
data {
  int n;    // number of obs
  int u;    // number of variables
  vector[n] y;
  matrix[n,u] x;
}
parameters {  // all except v will get uniform prior, which is default
 real cn;
 real<lower=-6, upper = 6> logs;   //log of s, related to lambda, not too high
 real<lower=-6, upper = 6> logsig;   //log of sig
 vector[u] v; //parameters to fit
}
transformed parameters {
 real s;                 // shrinkage parameter
 real sig;   //sigma
 vector[n] mu;  //means
 s = exp(logs);
 sig = exp(logsig);
 mu = cn+x*v;
}
model {  // gives priors for those not assumed uniform. Choose this one for Bayesian ridge regression.
   for (i in 1:u)  v[i] ~ normal(0, s);  // more weight to close to 0
  y ~ normal(mu,sig);
}
generated quantities { //outputs log likelihood for computing loo
  vector[n] log_lik;
 for (j in 1:n) log_lik[j] = normal_lpdf(y[j] | mu[j], sig);
}
```

The code including an age-year interaction term starts with two design matrices – one for cohorts and ages, in the rows and columns of the original dataset, and one for ages and year, the columns and diagonals. That one is later split into the two components, where the column factors are the trend weights applied to the year trends by age. The trend weights are standardized to be positive with a maximum at 1.0. The code here includes the log link and the gamma with variance proportional to mean. It is called lc for Lee-Carter.

```
dmat = as.matrix(read_excel('dsgn_tri_row_col.xlsx'))
coldiag = as.matrix(read_excel('dsgn_tri_col_diag.xlsx'))
y = scan('comp_log_y.txt')
dml = dmat[,-14]
cols = c(1:14)
diags = c(15:28)
diagm = coldiag[,diags]
wghtm = coldiag[,cols]
n <- ncol(diagm)
```

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```
u <- ncol(wghtm)
c(n,u)
N <- nrow(dml)
U <- ncol(dml)
c(N,U)
yy = exp(y)
df = list(N=N,U=U,dmat=dml,n=n,u=u,diagm=diagm,wghtm=wghtm,y=yy) #now run stan
set.seed(4)
fit_5 <- stan(file = 'ln_tri_spline_lc.stan', data=df, verbose = FALSE, chains = 1, iter = 10000, control =
 list(adapt_delta = 0.94, max_treedepth = 20))
```

This is the Stan code `'ln_tri_spline_lc.stan'`.

```
data {
  int N;          //number of observations
  int U;          //number of variables
  matrix[N,U] dmat;  //row col design matrix with U columns
  int n;          //number of diag params
  int u;          //number of wghts params
  matrix[N,n] diagm;  //diag design matrix
  matrix[N,u] wghtm;  //col wght dsgn mat
  vector[N] y;     //the triangle listed in a column
}
parameters {  // all except v will get uniform prior, which is default
 real<lower=-20, upper=20> lncn;//ln constant term, starting in known range
  vector[U] v;   //row-col parameters
  vector[u] w;  //trend-wghts parameters
  vector[n] d;  //diag parameters
 real<lower=-5, upper = 5> logs;     //log of s, related to lambda, not too high
 real<lower=-20, upper = 20> logbeta;   //log of gamma b parameter
}
transformed parameters {
 real beta;                      //variance in Stan = mean/beta
 real s;                        //shrinkage parameter, like lambda
 vector[N] alpha;                //fitted alpha parameter vector
 real cn;
 real m;  // max weight
 vector[N] colwghts;
 vector[N] trend;
 vector[N] yhat;
 beta = exp(logbeta);
 s = exp(logs);       // Gives more weight to lower values, which is good if X not big
 cn = exp(lncn);
 colwghts = wghtm*w;
```

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```
 m = max(colwghts);
 colwghts = exp(colwghts-m); //makes max = 1, all >0
 trend = diagm * d;
 for (j in 1:N) trend[j] = trend[j]*colwghts[j];
 yhat = exp(trend+dmat*v+cn);
 alpha = yhat*beta; //In Stan, mean = a/b
}
model {  // gives priors for those not assumed uniform. Choose this one for lasso.
   for (i in 1:U)  v[i] ~ student_t(2, 0, s);
   for (i in 1:u)  w[i] ~ student_t(2, 0, s);
   for (i in 1:n)  d[i] ~ student_t(2, 0, s);
for (j in 1:N) y[j] ~ gamma(alpha[j], beta);  //Stan gamma mean is a/b
}
generated quantities { //outputs log likelihood for looic
  vector[N] log_lik;
for (j in 1:N) log_lik[j] = gamma_lpdf(y[j] | alpha[j],beta);
}
```