Efficient Bayesian Regularization by Kalman Folding

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Abstract

We show, by numerical examples, that Kalman folding (KAL) produces the same results as recurrent least squares (RLS) and maximum a-posteriori (MAP), for appropriate choices of a-priori covariances, i.e., regularization hyperparameters. KAL and RLS are more intuitive than MAP for practical applications, plus offer space-time efficiency over MAP by avoiding storage and multiplication of large matrices. Because RLS and KAL are overt recurrences, a-priori data are necessary to bootstrap them, so regularization is naturally built-in to the formulation: they are Bayesian by construction. Contrast MAP, wherein a-priori belief is introduced as a Bayesian modification of traditional, maximum-likelihood (MLE) least-squares through the normal equations.

We exploit the novel fact that MAP is invariant when its hyperparameters are both swapped and inverted. After that transformation, the MAP equations strongly resemble the equations of Kalman filtering. This resemblance may suggest a future, general proof of the invariance, perhaps by conversion of MAP from explicit to recurrent form.

Introduction

Linear systems appear everywhere, and, where they don't appear naturally, linear approximations abound because non-linear systems are often intractable. Examples comprise machine learning, control, dynamics, robotics, and many more.

Linear regression is the standard technique for estimating coefficients or *parameters* of a linear model from given data. Often, authors sweep linear regression under the rug, presumably because readers know all about it. However, time and again, I see the normal equations directly applied (fat, slow, over-fitting), matrices inverted (risky), and neural networks applied (overkill).

Over-fitting is another hazard. Linear models, as their *order* (number of parameters) nears or exceeds the number of data points, tend to follow data too well, limiting smoothness and predictive power outside the bounds of the data. Models that over-fit "wiggle" too much and *generalize* poorly.

Regularization is the usual mitigation of over-fitting. In Bayesian MAP, regularization is introduced through a-priori *belief* hyperparameters α and β, the reciprocal variance of an a-priori estimate of the unknown parameters of the model, and the variance of the observations from the model, respectively.

We show here, numerically, that MAP produces the same results when α and β are swapped and inverted. After that transformation, the MAP equations strongly resemble the equations of Kalman filtering, promoting intuition in applications. Applied directly, rather than as reciprocals, and in opposite positions from MAP, these variances are concrete and can be estimated or learned directly from experimental conditions.

RLS and KAL also offer scaling advantages over MAP (see Beckman's series on Kalman folding at https://-goo.gl/iTxTzs). MAP is a modification of the *normal equations* of maximum-likelihood (MLE) regression. The normal equations and the MAP equations suggest explicit computation over whole data sets. There is no obvious way to convert them into recurrences. RLS and KAL, however, overtly process data one observation at a time, avoiding storage and multiplication of large matrices. RLS and KAL have natural expressions as *functional folds*, fitting into contemporary programming languages.

Motivating Review

First, we exhibit maximum-likelihood estimation (MLE) for a problem of order two: estimating the slope and intercept of a best-fit line to noisy data. This example puts an elementary problem into a setting that we generalize to higher order below. Furthermore, MLE *operates over all the data at once*, requiring matrices full of data to be stored, multiplied, and inverted. Not until we get to RLS and KAL do we see approaches much more efficient in memory and time.

MLE is computed four ways:

1. using Wolfram built-in functions

2. directly through the classic normal equations

3. using the Moore-Penrose left pseudoinverse

4. sidestepping the risky inverse by solving a linear system

These methods of MLE yield exactly the same results for this small example. It is easy to make them diverge numerically for models with more parameters, that is, of larger order.

■ Problem Statement

Find best-fit, unknown parameters m (slope) and b (intercept), where $z = m\,x + b$, given known, noisy data $(z_1,\ z_2,\ \ldots,\ z_N)$ and $(x_1,\ x_2,\ \ldots,\ x_N)$.

Write this *system* as a matrix equation and remember the symbols Z (*observations*, known), A (*partials*, known), and Ξ (*model, state, unknown parameters* to be estimated).

Rows of Z and A come in matched pairs.

$$Z_{N \times 1} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{pmatrix} = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{pmatrix} \cdot \begin{pmatrix} m_{unknown} \\ b_{unknown} \end{pmatrix} + \text{noise} \tag{1}$$

$$= A_{N \times 2} \cdot \Xi_{2 \times 1} + \text{samples of NormalDistribution}[0, \sigma_Z]$$

Ground Truth

Fake some data by (1) sampling a line specified by ground truth m and b, then (2) adding Gaussian noise. Run the faked data through the four estimation procedures and see how close the estimated $m_{estimated}$ and $b_{estimated}$ come to the ground truth.

In real-world applications, we rarely have ground truth. Its purpose is to baseline or calibrate the various methods.

In[1]:=
```
ClearAll[groundTruth, m, b];
groundTruth = {m, b} = {0.5, -1. / 3.};
```

Partials

The partials A are a (order-N column) vector of covectors (order-M row vectors). Each covector is the gradient 1-form of $A \cdot \Xi$ with respect to Ξ, evaluated at specific values of Ξ from the data. Gradients are best viewed as 1-forms, always covectors: linear transformations of vectors.

In[3]:=
```
ClearAll[nData, min, max];
nData = 119; min = -1.; max = 3.;
ClearAll[partials];
partials = Array[{#, 1.0} &, nData, {min, max}];
Short[partials, 3]
```

Out[7]//Short=
```
{{-1., 1.}, {-0.966102, 1.}, {-0.932203, 1.},
  {-0.898305, 1.}, <<112>>, {2.9322, 1.}, {2.9661, 1.}, {3., 1.}}
```

■ Faked Observations Z

Here we define a global variable, **data**, to be used in later derivations and demonstrations:

In[8]:=
```
ClearAll[fake];
fake[n_, σ_, A_, {m_, b_}] :=
  Table[
    RandomVariate[NormalDistribution[0, σ]] + A〚i〛.{m, b},
    {i, n}];
```

In[10]:=
```
ClearAll[data, noiseσ];
noiseσ = 0.65;
data = fake[nData, noiseσ, partials, groundTruth];
Short[data, 3]
```

Out[13]//Short=
```
{-1.88854, -0.374884, -0.645932, -1.20269,
   ≪111≫, 0.35366, 0.523939, 2.20031, 2.0421}
```

■ Wolfram Built-In

The Wolfram built-in **LinearModelFit** computes an MLE (maximum-likelihood estimate) for Ξ. The estimated $m_{estimated}$ and $b_{estimated}$ are reasonably close to the ground truth $\begin{pmatrix} m \\ b \end{pmatrix} = \begin{pmatrix} 0.5 \\ -0.333333 \end{pmatrix}$.

In[14]:=
```
ClearAll[model];
model = LinearModelFit[{partials〚All, 1〛, data}ᵀ, x, x];
Normal[model]
```

Out[16]=
```
-0.385503 + 0.601925 x
```

Un-comment the following line to see everything Wolfram has to say about this MLE (it's a lot of data).

In[17]:=
```
(*Association[(#→model[#])&/@model["Properties"]]*)
```

For purposes below, the most important attribute of the model is its covariance matrix. We come back to it below.

In[18]:=
```
model["CovarianceMatrix"] // MatrixForm
```

Out[18]//MatrixForm=
$$\begin{pmatrix} 0.00667312 & -0.00283247 \\ -0.00283247 & 0.00283247 \end{pmatrix}$$

The plot shows that Wolfram does an acceptable job, for practical purposes, of estimating the parameters *m* and *b* that define the line. We have 119 data and two parameters to estimate, so over-fitting will not be an issue in this early example. We explore over-fitting at length below.

In[19]:=
```
Show[ListPlot[{partials〚All, 1〛, data}ᵀ],
  Plot[{m x + b, model[x]}, {x, min, max}]]
```

Out[19]=
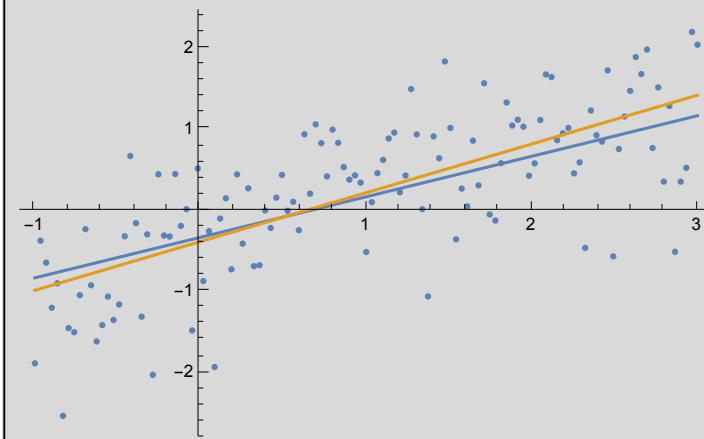
Normal Equations

Solve equation 1 for a value of Ξ that minimizes sum-squared error $J(\Xi) \stackrel{\text{def}}{=} (Z - A \cdot \Xi)^{\mathsf{T}} \cdot (Z - A \cdot \Xi)$. That is the same as maximizing the likelihood of the data given the parameters, $p(Z \mid \Xi)$. Because the noise $\mathcal{N}(0, \sigma)$ has zero mean, The solution turns out to be exactly what one would get from naive algebra: $A^{\mathsf{T}} \cdot A$ is square; when it is invertible,

$$(A^{\mathsf{T}} \cdot A)^{-1} \cdot A^{\mathsf{T}} \cdot Z = \Xi \tag{2}$$

That gives numerically the same answer as Wolfram's built-in:

In[20]:=
```
Inverse[partialsᵀ.partials].partialsᵀ.data
```

Out[20]=
```
{0.601925, -0.385503}
```

Moore-Penrose PseudoInverse

The matrix $(A^{\mathsf{T}} \cdot A)^{-1} \cdot A^{\mathsf{T}}$ is the *Moore-Penrose left pseudoinverse*. Wolfram has a built-in for it. We get exactly the same answer as above:

In[21]:=
```
PseudoInverse[partials].data
```

Out[21]=
```
{0.601925, -0.385503}
```

Avoiding Inversion

Avoid the inverse via **LinearSolve**. We have more to say about avoiding inverses below.

In[22]:=
```
LinearSolve[partialsᵀ.partials, partialsᵀ].data
```

Out[22]=
```
{0.601925, −0.385503}
```

Don't Use the Normal Equations

$(A^\mathsf{T} \cdot A)^{-1} \cdot A^\mathsf{T} \cdot Z$ is a nasty computation: in memory usage (big matrices), in time (matrix multiplication), and in numerical risk (inverse). How to avoid these hazards? Find a recurrence relation.

Recurrence

Fold this recurrence over Z and A:

$$\xi \leftarrow (\Lambda + a^\mathsf{T} \cdot a)^{-1} \cdot (a^\mathsf{T} \cdot \zeta + \Lambda \cdot \xi)$$
$$\Lambda \leftarrow (\Lambda + a^\mathsf{T} \cdot a)$$

(3)

where

- ξ is the current estimate of Ξ

- a and ζ are matched rows of A and Z

- Λ accumulates $A^\mathsf{T} \cdot A$.

Derivation Sketch

Derive the recurrence as follows: Treat the estimate-so-far,

$$\xi_{\text{so-far}} \overset{\text{def}}{=} (A^\mathsf{T} \cdot A)^{-1} \cdot A^\mathsf{T} \cdot Z_{\text{so-far}}$$

(4)

as just one more observation with information matrix

$$\Lambda = A_{\text{so-far}}{}^\mathsf{T} \cdot A_{\text{so-far}}$$

(5)

The scalar *performance* or *squared error* of the estimate, so far, is

$$J(\xi) \;=\; (Z_{\text{so-far}} - A_{\text{so-far}} \cdot \xi)^\mathsf{T} \cdot (Z_{\text{so-far}} - A_{\text{so-far}} \cdot \xi) \;=\; (\xi - \xi_{\text{so-far}})^\mathsf{T} \cdot \Lambda \cdot (\xi - \xi_{\text{so-far}})$$

(6)

where ξ is the unknown true parameter vector, $Z_{\text{so-far}}$ is the column vector of all observations so-far, and $\Lambda = A_{\text{so-far}}{}^\mathsf{T} \cdot A_{\text{so-far}}$. Adding a new observation, ζ and its corresponding partial row covector a, increases

the error $J(\xi)$ by $(\zeta - a \cdot \xi)^{\mathsf{T}} \cdot (\zeta - a \cdot \xi)$. Minimize the new total error with respect to ξ to find the recurrence (exercise). ∎

We see that RLS perforce introduces an a-priori estimate ξ_0 and its covariance, which is the inverse of the information matrix Λ_0. RLS is Bayesian by construction. We show below that, when renormalized with an a-priori covariance for the observations ζ, is theoretically equivalent to KAL and numerically equivalent to MAP. Proof of theoretical equivalence to MAP awaits future work.

Numerical Demonstration

Bootstrap the recurrence with ad-hoc, a-priori values $\xi_0 = (\begin{matrix} 0 & 0 \end{matrix})^{\mathsf{T}}$ and $\Lambda_0 = ((\begin{matrix} 10^{-6} & 0 \end{matrix})(\begin{matrix} 0 & 10^{-6} \end{matrix}))$.

In[23]:=
```
ClearAll[update];
update[{ξ_, Λ_}, {ζ_, a_}] :=
  With[{Π = (Λ + aᵀ.a)},
    {Inverse[Π].(aᵀ.ζ + Λ.ξ), Π}];

MatrixForm /@
  ({{(mBar
      bBar), Π} =
    Fold[update, {(0
                   0), (1.0*^-6      0
                        0        1.0*^-6)},
    {List /@ data, List /@ partials}ᵀ])
```

Out[25]=
$$\left\{ \begin{pmatrix} 0.601925 \\ -0.385503 \end{pmatrix}, \begin{pmatrix} 280.356 & 119. \\ 119. & 119. \end{pmatrix} \right\}$$

The estimates **mBar** and **bBar** are, numerically, the same as we got from Wolfram's built-in. For this example, the choice of ξ_0 and Λ_0 had negligible effect.

Structural Notes

The mappings of **List** over the data and partials convert them into column vectors. Wolfram built-ins and the normal equations, implicitly, treat one-dimensional lists as columns or rows as needed, then compute inner (dot) products as if the distinction did not matter. Python's numpy has the same dubious feature.

Memory and Time Efficiency

The required memory for the recurrence is $O(M)$, where M is the order of the model, the number of parameters to estimate, the length of Ξ, and the length of each row of A. There is no dependency at all on the number N of data items. Also, the recurrence accumulates data one observation at a time, and is thus $O(N)$ in time. Contrast with the normal equations, which multiply at $\sim O(N^3)$ and invert at $\sim O(M)$, i.e., at much

greater time cost.

Check the A-Priori

The final value of Λ (called Π in the code, a returned value), is $A_{full}{}^{\intercal} \cdot A_{full} + \Lambda_0$. To check the code, check that the difference between Π and $A_{full}{}^{\intercal} \cdot A_{full}$ is Λ_0:

In[26]:=
```
Π - partialsᵀ.partials
```

Out[26]=
$$\{\{1. \times 10^{-6}, 0.\}, \{0., 1. \times 10^{-6}\}\}$$

Covariance of the Estimate

The covariance of this estimate Ξ is $\left(\frac{n-1}{n-2}\right) * \text{Variance}[Z - A \cdot \Xi] * \Lambda^{-1}$ except for a small contribution from the a-priori information Λ_0. The correction factor $\left(\frac{n-1}{n-2}\right)$ is a generalization of Bessel's correction. The 2 in $(n-2)$ in the denominator of Bessel's correction is the number of parameters being estimated (see VAN DE GEER, Least Squares Estimation, Volume 2, pp. 1041–1045, in Encyclopedia of Statistics in Behavioral Science, Eds. Brian S. Everitt & David C. Howell, Wiley, 2005). The denominator of the correction, in general, is $n - p$, where n is the number of data and p is the number of parameters being estimated.

In[27]:=
```
Inverse[partialsᵀ.partials] * nData - 1
                             ──────────  *
                             nData - 2

   Variance[data - partials.{mBar, bBar}] // MatrixForm
```

Out[27]//MatrixForm=
$$\begin{pmatrix} 0.00283247 & -0.00283247 \\ -0.00283247 & 0.00667312 \end{pmatrix}$$

Except for the reversed order, this is the same covariance matrix that Wolfram's **LinearModel** reports:

In[28]:=
```
Reverse@(Reverse /@ model["CovarianceMatrix"]) // MatrixForm
```

Out[28]//MatrixForm=
$$\begin{pmatrix} 0.00283247 & -0.00283247 \\ -0.00283247 & 0.00667312 \end{pmatrix}$$

■ Don't Invert That Matrix

See https://www.johndcook.com/blog/2010/01/19/dont-invert-that-matrix/

In general, replace any occurrence of $A^{-1} \cdot B$ or **Inverse[A].B** with **LinearSolve[A,B]** for arbitrary square matrix A and arbitrary matrix B. Almost all programming languages and toolkits support an efficient and robust analogue to Wolfram's **LinearSolve**.

In[29]:=
```
ClearAll[update];
update[{ξ_, Λ_}, {ζ_, a_}] :=
  With[{Π = (Λ + aᵀ.a)},
    {LinearSolve[Π, (aᵀ.ζ + Λ.ξ)], Π}];


MatrixForm /@ ({{(mBar
                   bBar), Π} =
    Fold[update, {(0
                   0), (1.0*^-6     0
                        0      1.0*^-6)},
     {List /@ data, List /@ partials}ᵀ]})
```

Out[31]=
$$\left\{ \begin{pmatrix} 0.601925 \\ -0.385503 \end{pmatrix}, \begin{pmatrix} 280.356 & 119. \\ 119. & 119. \end{pmatrix} \right\}$$

Because this example is small, **Inverse** has no obvious numerical issues. It is very easy to produce large, ill-conditioned matrices, and one will spend a lot of time and storage inverting them, only to get useless results.

■ Interim Conclusions

We have eliminated memory bloat by processing updates one observation at a time, each with its paired partial. We reduce computation time and numerical risk by solving a linear systems instead of inverting a matrix. We also avoid multiplication of $O(N)$ matrices, which is of approximately $O(N^3)$ time.

Sidebar: Estimating 1-Forms (Gradients)

In linear algebra, vectors are conventionally columns, i.e., $n \times 1$ matrices, and covectors are rows, i.e., $1 \times n$ matrices (see Vector Calculus, Linear Algebra, and Differential Forms, A Unified Approach by John H. Hubbard and Barbara Burke Hubbard). In this language, *dual* means *transpose*.

When the model --- the thing we're estimating --- is a covector (row-vector), e.g., a 1-form, we have the dual (transposed) problem to the one above. This situation arises in reinforcement learning by policy gradient. In that case, the observations Ω and the model Γ are now covectors with elements ω and γ instead of ζ and ξ. The co-partials Θ (replacing A) are now a covector of column vectors θ. The observation equation is $\Omega = \Gamma \cdot \Theta$ and the error-so-far is $(x - \gamma) \cdot \Lambda \cdot (x - \gamma)^\intercal$, where $\Lambda = \Theta_{so-far} \cdot \Theta_{so-far}^\intercal$. We don't change the name of Λ because it's symmetric. Adding a new observation ω introduces new error $(\omega - x \cdot \theta) \cdot (\omega - x \cdot \theta)^\intercal$. Minimizing the total error yields

$$\gamma \leftarrow (\gamma \cdot \Lambda + \omega \cdot \theta^\intercal).(\Lambda + \theta \cdot \theta^\intercal)^{-1}$$
$$\Lambda \leftarrow (\Lambda + \theta \cdot \theta^\intercal)$$

(7)

straight transposes of equation 3. **LinearSolve** operates on the transposed right-hand side of the recurrence, and we transpose the solution to get the recurrence. We apply this dual model to the transpose of the original data:

```
In[32]:=   Short[Transpose /@ List /@ partials, 3]
```

```
Out[32]//Short=   {{{-1.}, {1.}}, {{-0.966102}, {1.}}, {{-0.932203}, {1.}},
     ≪113≫, {{2.9322}, {1.}}, {{2.9661}, {1.}}, {{3.}, {1.}}}
```

```
In[33]:=   ClearAll[coUpdate];
           coUpdate[{γ_, Λ_}, {ω_, θ_}] :=
             With[{Π = (Λ + θ.θᵀ)},
               {LinearSolve[Π, Λ.γᵀ + θ.ωᵀ]ᵀ, Π}];
           MatrixForm /@ Fold[coUpdate,
             {( 0  0 ), ( 1.0*^-6      0
                           0       1.0*^-6 )},
             {List /@ List /@ data, Transpose /@ List /@ partials}ᵀ]
```

```
Out[35]=   {( 0.601925  -0.385503 ), ( 280.356  119.
                                        119.    119. )}
```

■ Application of the Dual Problem

The finite-difference method of policy-gradient machine learning provides an example of this dual problem (see http://www.scholarpedia.org/article/Policy_gradient_methods).

Imagine a scalar function $J(\theta)$ of a column K-vector $\theta_{K \times 1}$. We want to estimate its gradient covector $\nabla_\theta J$, given a batch of $\mathcal{I}$ random increments $\Delta\Theta_{K \times \mathcal{I}}$, from the system $\nabla_\theta J \cdot \Delta\Theta = \Delta J$. Here, $\nabla_\theta J$ takes the role of the model whose state parameters Γ we want to estimate, $\Delta\Theta$ takes the role of the partials of the model w.r.t. those parameters, and ΔJ takes the role of measured data. Let $\Delta J_{\mathcal{I} \times 1}$ be a *batch* of observed increments to J and $\Delta\Theta_{K \times \mathcal{I}}$ be a matrix of the $\mathcal{I}$ corresponding column-vector random increments to the input vectors $\theta_{K \times 1}$. The right pseudoinverse $\mathrm{RPI} \overset{\text{def}}{=} (\Delta\Theta_{K \times \mathcal{I}} \cdot \Delta\Theta_{K \times \mathcal{I}}^{\mathsf{T}})^{-1} \cdot \Delta\Theta_{K \times \mathcal{I}}^{\mathsf{T}}$ solves $\nabla_\theta J_{\mathcal{I} \times 1} \cdot \Delta\Theta_{K \times \mathcal{I}} = \Delta J_{\mathcal{I} \times 1}$ to yield $\nabla J_{\mathcal{I} \times 1} \approx \Delta J_{\mathcal{I} \times 1} \cdot \mathrm{RPI}$.

Instead of the pseudoinverse, which is large, slow, and risky, use the co-update recurrence for this problem.

Regularization By A-Priori

Chris Bishop's *Pattern Recognition and Machine Learning* has an extended example fitting higher-order polynomials, linear in their coefficients, starting in section 1.1. The higher the order of the polynomial, the

more MLE over-fits. Bishop presents MAP regularization as a cure for this over-fitting. RLS and KAL already regularize, by construction. In this section, we relate their regularization to MAP's.

RLS and KAL each require an a-priori estimate of the unknown parameters and an a-priori uncertainty of that estimate to bootstrap recurrences. RLS takes the uncertainty as an *information matrix*. KAL takes the uncertainty as a *covariance matrix*. KAL additionally requires an estimate of observation noise, which arises in real problems and can often be estimated out-of-band. We show that RLS can and should be renormalized with observation noise to produce results equivalent to KAL and MAP.

■ Reproducing Bishop's Example

Bishop's Training Set

First, create a sequence of N = 10 inputs for a *training set*, equally spaced in [0 .. 1].

In[36]:=
```
ClearAll[bishopTrainingSetX];
bishopTrainingSetX[N_] := Array[Identity, N, {0., 1.}];
ListPlot[bishopTrainingSetX[10]]
```

Out[38]=
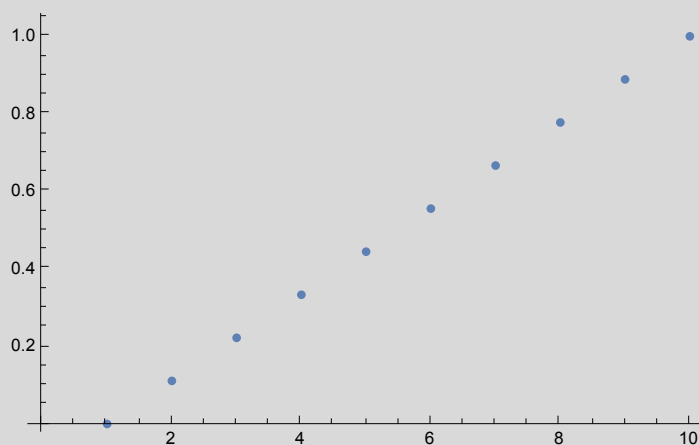
Bishop's ground truth is a single cycle of a sine wave. Add noise to a sample taken at the inputs of the training set above. Bishop doesn't state his observation noise, but I guess $\sigma_z = \sigma_t = 0.30$ to create a fake data set that resembles Bishop's qualitatively.

Wolfram's built-in **NormalDistribution** takes the standard deviation as its second argument, not the variance. Mixing up standard deviation and variance is an easy mistake. Bishop's notation for normal distribution takes variance as second argument, so beware.

In[39]:=
```
ClearAll[bishopTrainingSetY, bishopGroundTruthY];
bishopGroundTruthY[xs_] := Sin[2. π #] & /@ xs;
bishopTrainingSetY[xs_, σ_] :=
  With[{n = Length@xs},
    bishopGroundTruthY[xs]
      + RandomVariate[NormalDistribution[0., σ], n]];
```

Take a sample of the outputs and assign it the names **bts** for **bishopTrainingSet**. It isn't his actual training set, which I didn't find in print, just my simulation.

In[42]:=
```
ClearAll[bishopTrainingSet, bts, bishopFake, bishopFakeSigma];
bishopFake[n_, σ_] :=
  With[{xs = bishopTrainingSetX[n]},
    With[{ys = bishopTrainingSetY[xs, σ]},
      {xs, ys}]];
bishopFakeSigma = 0.30;
bishopTrainingSet = bts = bishopFake[10, bishopFakeSigma];
```

Make a plot like Bishop's figure 1.7 (page 10).

In[46]:=
```
With[{lp = ListPlot[btsᵀ,
      PlotMarkers → {Graphics@{Blue, Circle[{0, 0}, 1]}, .05}]},
 Show[{lp, (* once to set the scale *)
   Plot[Sin[2. π x], {x, 0., 1.}, PlotStyle → {Thick, Green}],
   lp (* again to overdraw the plot *)},
  Frame → True,
  FrameLabel → {"x", "t"}]]
```

Out[46]=
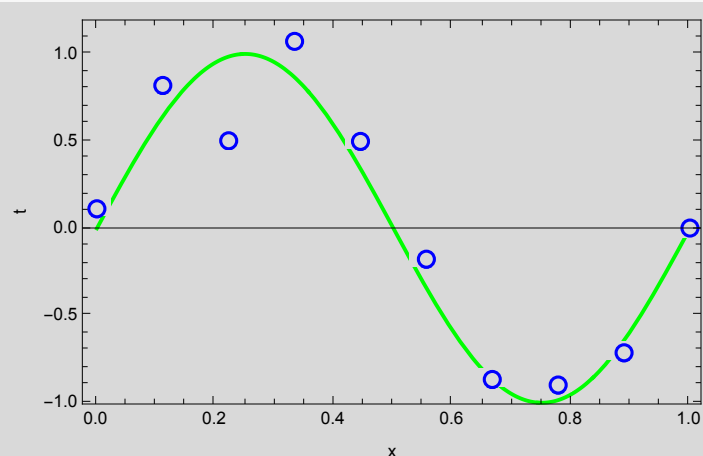
Partials: Gradients of the Unknown Parameters

Write a function for partials. Quietly map the indeterminate 0^0 to 1. Test it symbolically.

In[47]:=
```
ClearAll[partialsFn];
partialsFn[order_, xs_] :=
   Transpose@Quiet@Table[#^(i-1) /. {Indeterminate → 1}, {i, order + 1}] &@xs;
MatrixForm@partialsFn[6, {x₁, x₂, x_M}]
```

Out[49]//MatrixForm=

$$\begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 & x_1^4 & x_1^5 & x_1^6 \\ 1 & x_2 & x_2^2 & x_2^3 & x_2^4 & x_2^5 & x_2^6 \\ 1 & x_M & x_M^2 & x_M^3 & x_M^4 & x_M^5 & x_M^6 \end{pmatrix}$$

The MAP Equations

Confer Bishop's equation 3.3, page 138, where he writes the parameters to estimate as **w** and the observation equation as

$$y(\mathbf{x}, \ \mathbf{w}) = \sum_{j=0}^{M} w_j \, \phi_j(\mathbf{x})$$

(*bias* incorporated as coefficient w_0 of 0th basis function). This is predictive: you give me concrete inputs **x**, parameters **w**, and I'll give you a predicted observation y in terms of $M + 1$ basis functions ϕ corresponding to the $M + 1$ unknown parameters. For polynomial basis functions, the number of parameters is one more than the order M of the polynomials. The basis functions can be anything, however: wavelets, Fourier components, etc.

Bishop (inexplicably) converts **w** into a covector and writes

$$y(\mathbf{x}, \ \mathbf{w}) = \mathbf{w}^{\mathsf{T}} \, \phi(\mathbf{x})$$

where $\phi(\mathbf{x})$ is an $(M + 1)$-dimensional column-vector of basis functions, the transpose of one row of our partials matrix A. We claim it's better always to think of partials or gradients as values of differential forms, thus covectors (row vectors or covariant vectors, see https://goo.gl/DkeVmM, https://-goo.gl/JgzqLR, and https://goo.gl/4TcF4T).

To find best-fit values for **w**, rows of the partials matrix A are the covector gradients of y with respect to **w**. We prefer to write

- observations as an N-dimensional column-vector Z_N with elements $\zeta_{j \in [1..N]}$

- the model or unknown parameters, an $(M + 1)$-dimensional column-vector $\Xi_{(M+1) \times 1}$ with elements $\xi_{i \in [0..M]}$

- partials matrix as $A_{N\times(M+1)}$

Bishop calls our partials matrix the *design matrix* in his equation 3.16, page 142, consisting of values of the basis functions at the concrete inputs $x_{n\in[1..N]}$. Bishop must (more cumbersomely) work in the dual of our formulation.

We prefer to write as follows: the covector rows of the design matrix terms as polynomial basis functions evaluated at the input points $x_{n\in[1..N]}$:

$$Z \;=\; A\cdot\Xi \;=\; \begin{pmatrix} \zeta_0 \\ \zeta_1 \\ \vdots \\ \zeta_N \end{pmatrix} \;=\; \begin{pmatrix} 1=x_1^0 & x_1 & x_1^2 & \cdots & x_1^M \\ 1=x_2^0 & x_2 & x_2^2 & \cdots & x_2^M \\ \vdots & \vdots & & \ddots & \vdots \\ 1=x_N^0 & x_N & x_N^2 & \cdots & x_N^M \end{pmatrix} \cdot \begin{pmatrix} \xi_0 \\ \xi_1 \\ \vdots \\ \xi_M \end{pmatrix} \;+\; \text{noise} \tag{8}$$

then packed up into rows of the A matrix.

$$Z \;=\; A\cdot\Xi \;=\; \begin{pmatrix} \zeta_0 \\ \zeta_1 \\ \vdots \\ \zeta_N \end{pmatrix} \;=\; \begin{pmatrix} A_{1\times(M+1)}(x_1) \\ A_{1\times(M+1)}(x_2) \\ \vdots \\ A_{1\times(M+1)}(x_N) \end{pmatrix}_{N\times(M+1)} \cdot \begin{pmatrix} \xi_0 \\ \xi_1 \\ \vdots \\ \xi_M \end{pmatrix} \;+\; \text{noise} \tag{9}$$

MLE: The Normal Equations

Mechanize the normal equations for comparison purposes; we expect them to over-fit.

```
In[50]:=   ClearAll[mleFit];
           mleFit[M_, trainingSet_] :=
              With[{xs = trainingSet[[1]], ys = trainingSet[[2]]},
                 PseudoInverse[partialsFn[M, xs]].ys];
           mleFit[3, bts]
```

```
Out[52]=   {0.0390293, 9.61433, -28.6574, 18.9797}
```

A convenience function:

```
In[53]:=   ClearAll[symbolicPowers];
           symbolicPowers[variable_, order_] :=
              partialsFn[order, {variable}][[1]];
```

The normal equations as a symbolic polynomial. Notice we can increase the order beyond the number of data, creating an underdetermined system. This is not the typical case in real-world data processing. Usually the number of data exceed the order and the system is overdetermined. The pseudoinverse is agnostic to the distinction.

```
In[55]:=    ClearAll[x];
            Manipulate[
             symbolicPowers[x, M].mleFit[M, bts],
             {{M, 3, "polynomial order M"}, 0, 16, 1, Appearance → {"Labeled"}}]
```

Out[56]=

polynomial order M ———————■ 3

$$0.0390293 + 9.61433\,x - 28.6574\,x^2 + 18.9797\,x^3$$

RLS: Recurrent Least Squares

RLS is regularized by its a-priori estimate of the unknown parameters and its a-priori information matrix. Use the slider below to see that once the minimum info becomes too large, the Λ matrix becomes ill-conditioned: pink warning message appear from the Wolfram kernel, and the solution is numerically suspect. In the rest of this paper, we eliminate these error message by applying Wolfram's **Quiet** because we notice, numerically, that ill-conditioning of the information matrix does not seem to be harmful.

```
In[57]:=    ClearAll[rlsFit];
            rlsFit[σ2Λ_][M_, trainingSet_] :=
              With[{xs = trainingSet〚1〛, ys = trainingSet〚2〛},
                With[{ξ0 = List /@ ConstantArray[0, M + 1],
                  Λ0 = σ2Λ * IdentityMatrix[M + 1]},
                 Fold[update, {ξ0, Λ0},
                  {List /@ ys, List /@ partialsFn[M, xs]}ᵀ]]];

            Manipulate[
             rlsFit[10^(-logσ2Λ)][3, bts]〚1〛,
             {{logσ2Λ, 9.034}, 0, 16, Appearance → "Labeled"}]
```

Out[59]=

logσ2Λ ——————————■ 9.034

$$\{\{0.0390298\}, \{9.61432\}, \{-28.6574\}, \{18.9796\}\}$$

KAL: Foldable Kalman Filter

The foldable Kalman filter (KAL) follows below. This version has only the *update* phase of a typical Kalman filter because the parameters-to-estimate are constant and there is no *predict* phase.

Note the P_Z parameter, the first in the definition of **kalmanUpdate**. This is the *covariance matrix of the observation noise*. It is a constant throughout the folding run of the filter. That's why it's lambda-lifted into its own function slot; **kalmanUpdate**, called with some concrete value of P_Z, yields a function that can be folded over an a-priori estimate ξ_o and covariance P_o and a sequence of observation-and-partial-covector pairs $\{\zeta, a\}$.

In[60]:=
```
ClearAll[kalmanUpdate, kalFit];
kalmanUpdate[Pz_][{ξ_, P_}, {ζ_, a_}] :=
  Module[{D, KT, K, L},
    D = Pz + a.P.aᵀ;
    KT = LinearSolve[D, a.P]; K = KTᵀ;
    L = IdentityMatrix[Length[P]] – K.a;
    {ξ + K.(ζ – a.ξ), L.P}];

kalFit[σξ2_, σξ2_][order_, trainingSet_] :=
  With[{xs = trainingSet〚1〛, ys = trainingSet〚2〛},
    With[{ξ0 = List /@ ConstantArray[0, order + 1],
      P0 = σξ2 * IdentityMatrix[order + 1]},
     Fold[kalmanUpdate[σξ2 * IdentityMatrix[1]],
      {ξ0, P0},
      {List /@ ys, List /@ partialsFn[order, xs]}ᵀ]]];
```

See All Three

The following interactive demonstration shows **mleFit** (normal equations), **rlsFit** (recurrent least squares), and **kalFit** (Kalman folding) on Bishop's training set.

When the a-priori information matrix in RLS is 10^{-6}, and when the a-priori covariance of the a-priori estimate in KAL is 10^6, both RLS and KAL produce regularized fits. In contrast, the MLE over-fits a 9th-order polynomial by interpolating (going through) every data point because a 9th-order polynomial fits the ten data points exactly: the normal equations are neither overdetermined nor underdetermined at order nine, but accidentally constitute an exactly solvable linear system.

Increasing **–logΛ** *decreases* the (magnitude of the) a-priori information matrix in RLS, meaning that we have less Bayesian belief in the a-priori estimate of the unknown parameters. Increasing **logσξ2** *increases* the a-priori covariance of the estimate in KAL and similarly decreases belief in the a-priori estimate. They eventually both over-fit the data completely and align with MLE. Later, we show that MAP can be similarly made to over-fit. Run the polynomial order up to nine, then **–logΛ** and **logσξ2** all the way to the right, to their maximum values.

In[63]:=

```
Manipulate[
 Module[{x}, (* gensym: fresh variable name *)
  With[{
    terms = symbolicPowers[x, M],
    cs = ϕ[M] /@ List /@ bts〚1〛},
   With[{
     recurrent = Quiet@rlsFit[10^(-logΛ0)][M, bts],
     normal = mleFit[M, bts],
     kalman = kalFit[bishopFakeSigma^2, 10^(logσξ2)][M, bts]},
    With[{
      rlsFn = {terms}.recurrent〚1〛,
      mleFn = terms.normal,
      kalFn = {terms}.kalman〚1〛},
     With[{lp = ListPlot[bts^T,
         PlotMarkers → {Graphics@{Blue, Circle[{0, 0}, 1]}, .05}]},
      Module[{showlist =
         {lp, Plot[Sin[2. π x], {x, 0., 1.}, PlotStyle → {Thick, Green}]}},
       If[rlsQ, AppendTo[showlist, Plot[rlsFn, {x, 0, 1},
          PlotStyle → {Purple}]]];
       If[mleQ, AppendTo[showlist, Plot[mleFn, {x, 0, 1},
          PlotStyle → {Orange}]]];
       If[kalQ, AppendTo[showlist, Plot[kalFn, {x, 0, 1}, PlotStyle → {Cyan}]]];
       Quiet@Show[showlist, Frame → True, FrameLabel → {"x", "t"}]]]]]]],
 Grid[{
   {Grid[{{
       Button["RESET", (M = 9; logΛ0 = 3; logσξ2 = 3) &],
       Control[{{rlsQ, True, "RLS"}, {True, False}}],
       Control[{{kalQ, True, "KAL"}, {True, False}}],
       Control[{{mleQ, True, "MLE"}, {True, False}}]}}]},
   {Control[{{M, 9, "polynomial order"}, 0, 16, 1, Appearance → {"Labeled"}}]},
   {Control[{{logΛ0, 3, "-log a-priori info (RLS)"},
      0, 16, Appearance → "Labeled"}]}, {Control[
     {{logσξ2, 3, "log a-priori cov (KAL)"}, 0, 16, Appearance → "Labeled"}]}}]]
```

Out[63]=
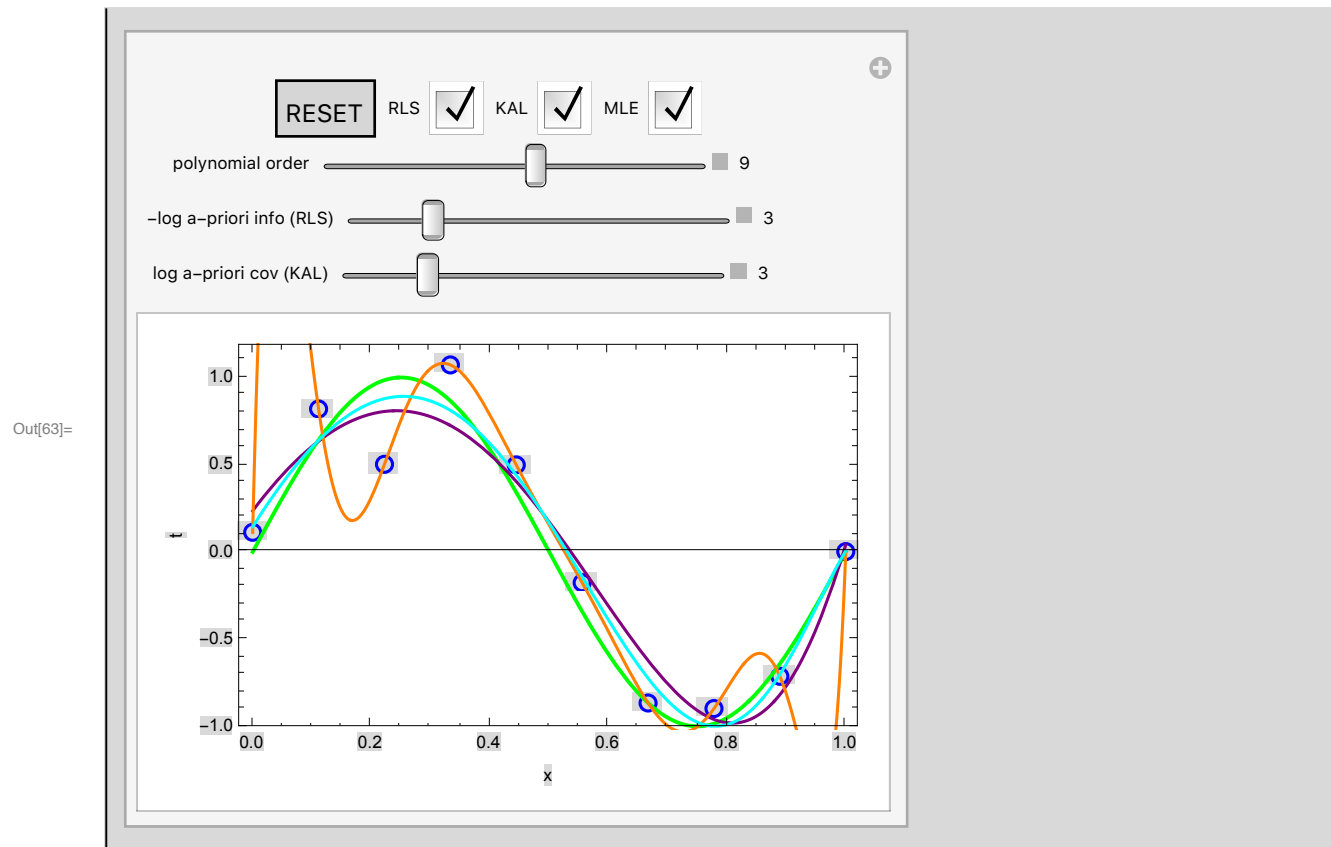
■ Renormalizing RLS

When the observation noise Z is unity, KAL coincides with RLS. In the demonstration below, a-priori information Λ in RLS is set always to be the inverse of a-priori estimate covariance *P* in KAL; RLS and KAL will have the same belief in the a-priori estimate of the unknown parameters. Vary the observation noise independently to see KAL and RLS coincide when it's zero.

As observation noise decreases, the solutions believe the observations more and the solution over-fits. As the a-priori covariance decreases, the solution believes the a-priori estimates more and the solution regularizes.

In[64]:=
```
Manipulate[Module[{x},
  With[{terms = symbolicPowers[x, M],
    cs = ϕ[M] /@ List /@ bts〚1〛},
   With[{rls = Quiet@rlsFit[10^(-2 logσξ)][M, bts],
     kalman = kalFit[10^(2 logσξ), 10^(2 logσξ)][M, bts]},
    With[{rlsFn = {terms}.rls〚1〛,
      kalFn = {terms}.kalman〚1〛},
     With[{lp = ListPlot[bts^T,
         PlotMarkers → {Graphics@{Blue, Circle[{0, 0}, 1]}, .05}]},
       Module[{showlist =
           {lp, Plot[Sin[2. π x], {x, 0., 1.}, PlotStyle → {Thick, Green}]}},
        If[rlsQ, AppendTo[showlist, Plot[rlsFn, {x, 0, 1},
           PlotStyle → {Purple}]]];
        If[kalQ, AppendTo[showlist, Plot[kalFn, {x, 0, 1}, PlotStyle → {Cyan}]]];
        Quiet@Show[showlist, Frame → True, FrameLabel → {"x", "t"}]]]]]],
  Grid[{{Grid[{{Button["RESET", (logσξ = 0.0; logσξ = 1.5; M = 9) &],
       Control[{{rlsQ, True, "RLS"}, {True, False}}],
       Control[{{kalQ, True, "KAL"}, {True, False}}]}}], ""},
    {Control[{{M, 9, "polynomial order"}, 0, 16, 1, Appearance → {"Labeled"}}],
     ""}, {Control[{{logσξ, 1.5, "log √P (KAL) = (-log √Λ ) (RLS) "},
       -3, 8, Appearance → "Labeled"}]},
    {Control[{{logσξ, 0.0, "log √z (KAL)"}, -6, 3, Appearance → "Labeled"}]}}]]]
```

Out[64]=
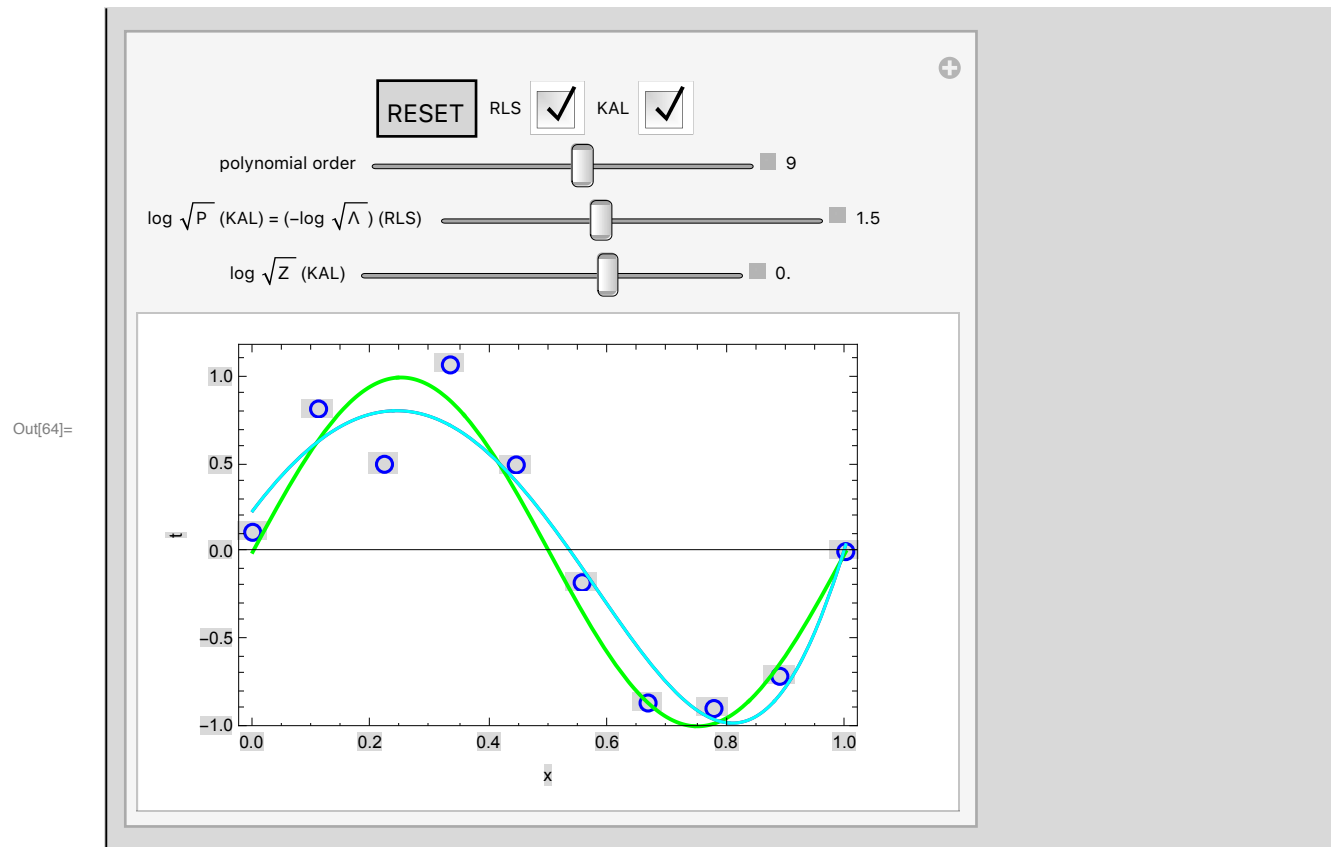
Add Observation Noise to RLS

RLS, so far, is normalized to unit observation (OBN) noise. How to modify RLS to account for non-normalized OBN noise?

Scale (each row of) the partials by the inverse of the OBN standard deviation, represented below by a matrix square root of the OBN covariance P_Z. Finally, rescale the final estimate (not the final covariance) by a matrix built from the inverse OBN standard deviation because the recurrent normal equations, which incrementally build $(P_Z^{-1} \cdot A^{\intercal} \cdot A \cdot P_Z^{-T})^{-1} \cdot P_Z^{-1} \cdot A^{\intercal} \cdot Z$, have one too many factors of P_Z.

```
In[65]:=   ClearAll[rlsUpdate];
           rlsUpdate[sqrtPz_][{ξ_, Λ_}, {ζ_, a_}] :=
             With[{sPzia = LinearSolve[sqrtPz, a]},
               With[{Π = (Λ + sPziaᵀ.sPzia)},
                 {LinearSolve[Π, (sPziaᵀ.ζ + Λ.ξ)], Π}]];


           Manipulate[
            With[{ξ0 = ( 0 ),  Λ0 = ( 1.0*^-6      0    ),
                        ( 0 )        (   0      1.0*^-6 )

              inputs = {List /@ data[[1 ;; n]], List /@ partials[[1 ;; n]]}ᵀ},

             Module[{ξrr, ξr, ξk, Πrr, Πr, Πk},

              ({ξrr, Πrr} = Fold[rlsUpdate[σ IdentityMatrix[1]],
                  {ξ0, Λ0}, inputs]);
              ({ξr, Πr} = Fold[update, {ξ0, Λ0}, inputs]);
              ({ξk, Πk} = Fold[kalmanUpdate[σ²], {ξ0, Inverse@Λ0}, inputs]);
              MatrixForm@{

                { IdentityMatrix[2] .ξrr, ξr, ξk}, {Πrr, Πr / σ², Inverse@Πk},
                  ───────────────
                        σ

                {Chop[Abs[Πrr - Πr / σ²], 10⁻⁶],
                  Chop[Abs[Inverse@Πk - Πr / σ²], 10⁻⁶],
                  Chop[Abs[Inverse@Πk - Πrr], 10⁻⁶]}}]],
            {{n, 3}, 3, nData, 1, Appearance → "Labeled"},
            {{σ, 1}, -100, 100, Appearance → "Labeled"}]
```
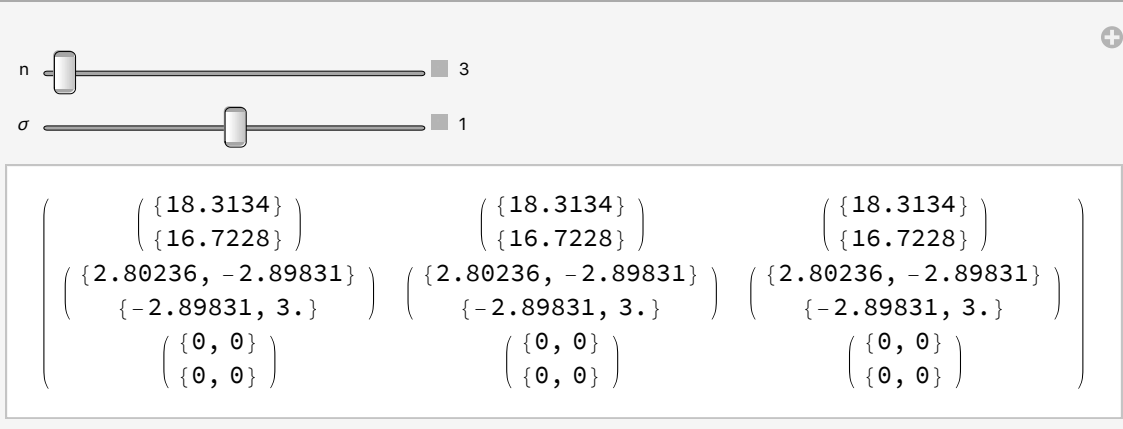


```
Out[67]=   ⎛      ( {18.3134} )           ( {18.3134} )           ( {18.3134} )     ⎞
           ⎜      ( {16.7228} )           ( {16.7228} )           ( {16.7228} )     ⎟
           ⎜ ( {2.80236, -2.89831} )  ( {2.80236, -2.89831} )  ( {2.80236, -2.89831} ) ⎟
           ⎜ (   {-2.89831, 3.}   )  (   {-2.89831, 3.}   )  (   {-2.89831, 3.}   ) ⎟
           ⎜       ( {0, 0} )            ( {0, 0} )            ( {0, 0} )      ⎟
           ⎝       ( {0, 0} )            ( {0, 0} )            ( {0, 0} )      ⎠
```

RLS beats KAL

KAL and renormalized RLS are mathematically equivalent. Operationally, KAL uses subtraction to recur the covariance of the estimates, so is exposed to catastrophic cancelation. RLS only adds to the information

matrix, so is exposed only to ill-conditioning, which is empirically less severe. We show this below.

Regularization and MAP

Bishop reports β = 11.111 … and α = 0.005 in his figure 1.17 (page 32) and in equations 1.70 through 1.72 (page 31), which look suspiciously like the equations for Kalman filtering. Bishop's matrix **S** looks like $\mathbf{D}^{-1}$ in **kalmanUpdate** above. Let's reproduce MAP via RLS and KAL.

■ Bishop's MAP

Bishop's equations 1.70 through 1.72 are reproduced here. The dimensions of the identity matrix in S is M + 1, where M is the order of the polynomial, one more than M to account for the leading bias term:

$$m(x) \;=\; \beta\,\phi(x)^{\intercal}\cdot S\cdot \sum_{n=1}^{N}\phi(x_n)\,t_n \tag{10}$$

$$s^2(x) \;=\; \beta^{-1} + \phi(x)^{\intercal}\cdot S\cdot \phi(x) \tag{11}$$

$$S^{-1} \;\stackrel{\mathrm{def}}{=}\; \alpha\,I_{M+1} + \beta\sum_{n=1}^{N}\phi(x_n)\cdot\phi(x_n)^{\intercal} \tag{12}$$

Here are links between Bishop's formulation and ours, without derivation.

$$\sum_{n=1}^{N}\phi(x_n)\,t_n = A^{\intercal}\cdot Z \tag{13}$$

$$\lim_{\alpha\to 0}\left(\beta^{-1}\,S^{-1}\right) = A^{\intercal}\cdot A \tag{14}$$

Φ Vectors

Bishop's $\phi(x_n)$ is a (M + 1)-dimensional column vector of the powers of the nth input x_n. These powers are the basis functions of a polynomial model for the curve. $\phi(x_n)$ is the dual (transpose) of one row of our partials matrix A.

As written, Bishop's equations are non-recurrent, requiring all data t_n and $\phi(x_n)$ in memory. Plus, as written, they require inverting matrix S. They thus suffer from the operational ills of the normal equations.

In[68]:=
```
ClearAll[ϕ];
ϕ[M_][xn_] := Quiet@Table[xn^i, {i, 0, M}] /. {Indeterminate → 1};
MatrixForm /@ ϕ[3] /@ List /@ bts[[1]]
```

Out[70]=
$$\left\{ \begin{pmatrix} 1 \\ 0. \\ 0. \\ 0. \end{pmatrix}, \begin{pmatrix} 1. \\ 0.111111 \\ 0.0123457 \\ 0.00137174 \end{pmatrix}, \begin{pmatrix} 1. \\ 0.222222 \\ 0.0493827 \\ 0.0109739 \end{pmatrix}, \begin{pmatrix} 1. \\ 0.333333 \\ 0.111111 \\ 0.037037 \end{pmatrix}, \begin{pmatrix} 1. \\ 0.444444 \\ 0.197531 \\ 0.0877915 \end{pmatrix}, \right.$$

$$\left. \begin{pmatrix} 1. \\ 0.555556 \\ 0.308642 \\ 0.171468 \end{pmatrix}, \begin{pmatrix} 1. \\ 0.666667 \\ 0.444444 \\ 0.296296 \end{pmatrix}, \begin{pmatrix} 1. \\ 0.777778 \\ 0.604938 \\ 0.470508 \end{pmatrix}, \begin{pmatrix} 1. \\ 0.888889 \\ 0.790123 \\ 0.702332 \end{pmatrix}, \begin{pmatrix} 1. \\ 1. \\ 1. \\ 1. \end{pmatrix} \right\}$$

S Inverse

Bishop's equation 1.72.

In[71]:=
```
ClearAll[sInv, α, β];
sInv[α_, β_, cs_, M_] :=
  With[{N = Length[cs]},
   α IdentityMatrix[M + 1] + β Sum[cs[[i]].cs[[i]]^T, {i, N}]];
```

MAP Mean

Bishop's equation 1.70.

In[73]:=
```
ClearAll[mapMean];
mapMean[α_, β_, x_, cs_, ts_, M_] :=
  With[{N = Length@cs},
    {β * ϕ[M][x]}.(* row of partials *)
     LinearSolve[(* vector of coefficients *)
      sInv[α, β, cs, M],
      ts.cs]][[1, 1]];
```

A-Priori Variances α and β

Bishop defines $\beta = 1/\sigma_\zeta^2$, where σ_ζ is the standard deviation, from the model, of the prediction ζ. The prediction ζ is the value of the model on an arbitrary input ξ. Similarly, Bishop defines $\alpha = 1/\sigma_\xi^2$, where σ_ξ is the standard deviation of the a-priori distribution of the unknown parameter estimate ξ.

We observe, numerically, that Bishop's equations match RLS and KAL when β is σ_ξ^2 and when $\alpha = \sigma_\zeta^2$. We

leave full proof to another paper, being satisfied with numerical evidence here.

Semi-numerically, the proposition is true (above order 4, The following becomes taxing for Mathematica):

In[75]:=
```
ClearAll[x, α, β, chopQ];
DynamicModule[{chopQ = False},
  Manipulate[With[{cs = φ[M] /@ List /@ bts[[1]], ts = bts[[2]]},
    If[chopQ, Chop, Identity]@
      FullSimplify[mapMean[α, β, x, cs, ts, M] - mapMean[1/β, 1/α, x, cs, ts, M]]],
    Column[{Row[{Button["UN-CHOP", chopQ = False], "          ",
      Button["CHOP", chopQ = True]}],
      Control[{{M, 2, "order M"}, 0, 4, 1, Appearance → {"Open", "Labeled"}}]}]]]
```

Out[76]=

UN–CHOP   CHOP

order M ———————●———————◼ 2

[2] — ▶ + ⌃ ⌄ →

$$
\begin{aligned}
&\Big(-7.8051 \times 10^{-17}\, \alpha^5 + \left(4.6861 \times 10^{-16} + 1.82001 \times 10^{-16}\, x^2\right) \alpha^4\, \beta + \\
&\quad \left(-8.56887 \times 10^{-15} + \left(2.14222 \times 10^{-15} - 1.56102 \times 10^{-16}\, x\right) x\right) \alpha^3\, \beta^2 + \\
&\quad \left(4.28444 \times 10^{-15} + \left(2.14222 \times 10^{-15} + 1.03448 \times 10^{-15}\, x\right) x\right) \alpha^2\, \beta^3 + \\
&\quad \left(-8.03332 \times 10^{-16} - 8.58561 \times 10^{-16}\, x\right) x\, \alpha\, \beta^4 + \\
&\quad \left(3.34722 \times 10^{-17} + \left(-2.00833 \times 10^{-16} + 1.84097 \times 10^{-16}\, x\right) x\right) \beta^5\Big) \Big/ \\
&\quad \left(\left(1.\, \alpha - 0.42885\, \beta\right)^2 \left(1.\, \alpha^3 + 15.8555\, \alpha^2\, \beta + 21.6818\, \alpha\, \beta^2 + 0.819658\, \beta^3\right)\right)
\end{aligned}
$$

The other two combinations, where $\beta = 1/\sigma_\zeta^2 \wedge \alpha = \sigma_\xi^2$ or $\beta = \sigma_\zeta^2 \wedge \alpha = 1/\sigma_\xi^2$ are not correct. Intuitively, these two combinations do not contain full information about the a-priori beliefs in both ζ and ξ, so we do not expect them to be correct. This fact can be demonstrated numerically.

In the following demonstration, the numerical evidence for equality of the two applications of MAP becomes overwhelming. MAP, RLS, and KAL match for all settings of σ_ξ^2, σ_ζ^2, M (order of the model), and assignments of α and β. The one deviation from perfect match concerns KAL. Explore the case where the order is around M = 4. For high σ_ξ^2 (don't believe the a-priori estimate of ξ) and low $\sigma_{\zeta z}^2$ (do believe the observational data), KAL fluctuates wildly. Why? The Kalman denominator $D = P_\zeta + a^\mathsf{T} P_\xi\, a$ becomes nearly $a^\mathsf{T} P_\xi\, a$. The Kalman gain, $K = P_\xi\, a^\mathsf{T} D^{-1}$ is nearly a^{-1}. The covariance update, $(I - K\, a) \cdot P$, becomes ill-conditioned, if not negative, because $K\, a$ is near unity.

Renormalized RLS does not suffer from these ills because it never subtracts. Renormalized RLS is still exposed to ill-conditioning of the information matrix, but that seems numerically to be less harmful to the final result. We wrap RLS in **Quiet** to suppress warnings. There is no free lunch; MAP also shows ill-conditioning and is similarly wrapped.

In[77]:=
```
ClearAll[rrlsFit];
rrlsFit[σ2ξ_, σ2ξ_][M_, trainingSet_] :=
  With[{xs = trainingSet[[1]], ys = trainingSet[[2]]},
   With[{ξ0 = List /@ ConstantArray[0, M + 1],
      Λ0 = σ2ξ^-1 * IdentityMatrix[M + 1]},
    Module[{ξ, Λ},
     {ξ, Λ} = Fold[
        rlsUpdate[√σ2ξ IdentityMatrix[1]],
        {ξ0, Λ0},
        {List /@ ys, List /@ partialsFn[M, xs]}ᵀ];
     {ξ / √σ2ξ , Λ}]]];
```

```
In[79]:=  DynamicModule[{αβBishop = True},
           Manipulate[Module[{x},
             With[{terms = symbolicPowers[x, M],
               cs = ϕ[M] /@ List /@ bts〚1〛, ts = bts〚2〛, σζ2 = 10.^2 logσζ, σξ2 = 10.^2 logσξ},
             With[{normal = mleFit[M, bts],
               kalman = kalFit[σζ2, σξ2][M, bts],
               rrls = Quiet@rrlsFit[σζ2, σξ2][M, bts]},
             With[{α = If[αβBishop, 1/σξ2, σζ2], β = If[αβBishop, 1/σζ2, σξ2]},
             With[{mleFn = terms.normal,
               kalFn = {terms}.kalman〚1〛,
               mapFn = Quiet@mapMean[α, β, x, cs, ts, M],
               rlsFn = {terms}.rrls〚1〛},
             With[{lp = ListPlot[btsᵀ,
                 PlotMarkers → {Graphics@{Blue, Circle[{0, 0}, 1]}, .05}]},
               Module[{showlist =
                 {lp, Plot[Sin[2. π x], {x, 0., 1.}, PlotStyle → {Thick, Green}]}},
                 If[mleQ, AppendTo[showlist, Plot[mleFn, {x, 0, 1},
                   PlotStyle → {Orange}]]];
                 If[rlsQ, AppendTo[showlist, Plot[rlsFn, {x, 0, 1},
                   PlotStyle → {Purple}]]];
                 If[kalQ, AppendTo[showlist, Plot[kalFn, {x, 0, 1},
                   PlotStyle → {Cyan}]]];
                 If[mapQ, AppendTo[showlist, Plot[mapFn, {x, 0, 1},
                   PlotStyle → {Magenta}]]];
                 Quiet@Show[showlist, Frame → True, ImageSize → Medium,
                   FrameLabel → {{"ζ", ""}, {"ξ", Grid[{{"α: ", α, "β:", β}}]
                     }}]]]]]]]],
             Column[{SetterBar[Dynamic[αβBishop],
               {True → "α = 1/σ_ξ²,  β = 1/σ_ξ²", False → "α = σ_ζ²,  β = σ_ξ²"}],
               Row[{Button["RESET", (M = 4; logσξ = .5; logσζ = -1.5) &],
                 Control[{{kalQ, True, "          KAL"}, {True, False}}],
                 Control[{{rlsQ, True, "          RLS"}, {True, False}}],
                 Control[{{mleQ, False, "           MLE"}, {True, False}}],
                 Control[{{mapQ, True, "          MAP"}, {True, False}}]}, Frame → All],
               Control[{{M, 4, "order M"}, 0, 16, 1, Appearance → {"Labeled"}}],
               Control[{{logσξ, .5, "log σξ (KAL)"}, -3, 5, Appearance → "Labeled"}],
               Control[{{logσζ, -1.5, "log σζ (KAL)"}, -7, 3, Appearance → "Labeled"}]}]]]
```

Out[79]=
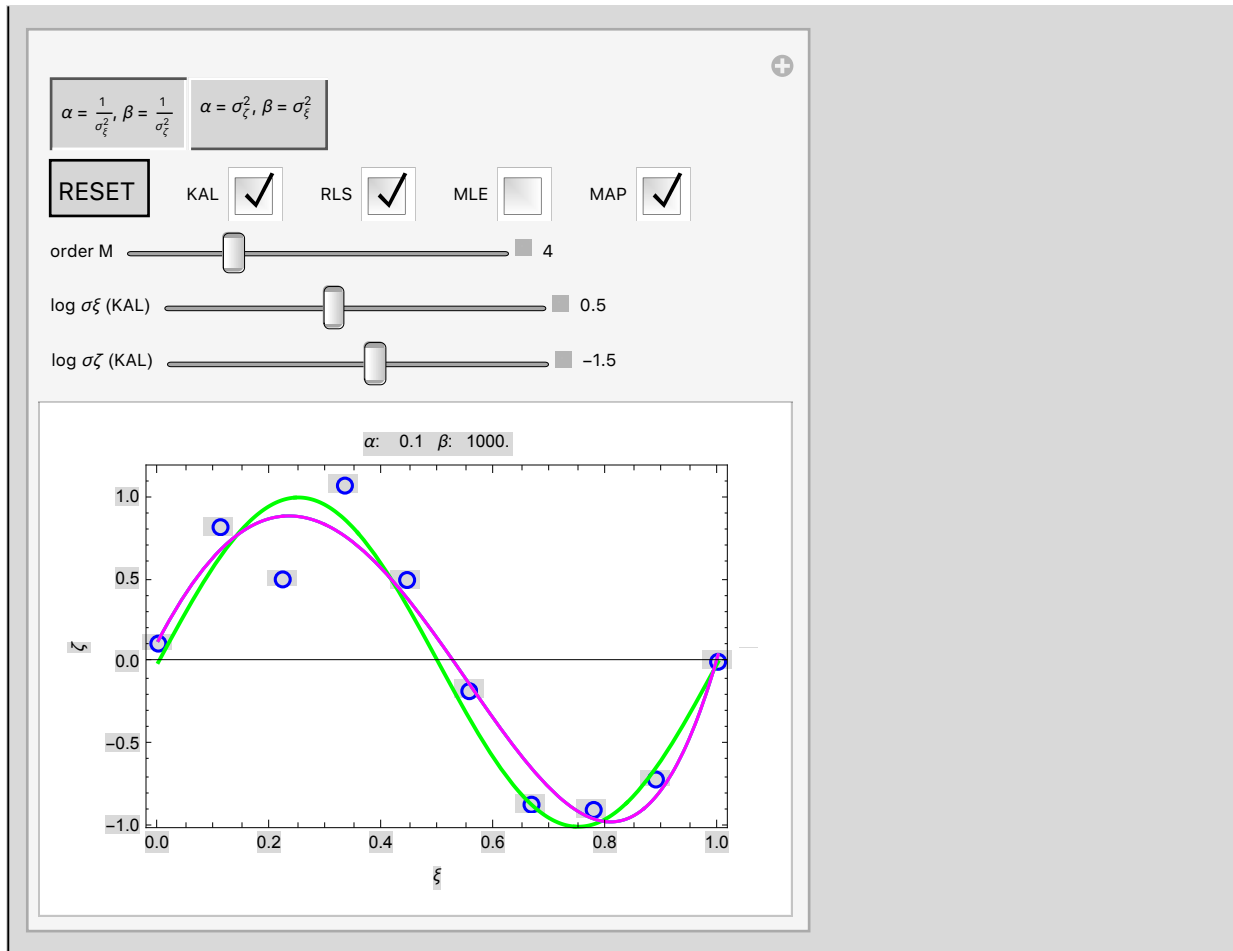
Covariance of the Estimate

Consider Bishop's equation 1.71 $s^2(x) = \beta^{-1} + \phi(x)^\intercal \cdot S \cdot \phi(x)$, which does not depend on the output data t_n, just as with KAL and RLS.

In[80]:=
```
ClearAll[mapsSquared];
mapsSquared[α_, β_, x_, cs_, M_] :=
  With[{a = ϕ[M][x]},
    β⁻¹ + {a}.LinearSolve[sInv[α, β, cs, M], List /@ a]];
```

Bishop kindly supplies the sigma-bars for his mean. He cites $\alpha = 0.005$ and $\beta = 11.1$, which correspond to $\sigma_\zeta = 0.07071$ and $\sigma_\xi = 3.333$, and $\log_{10} \sigma_\zeta = -1.15051$ and $\log_{10} \sigma_\xi = 0.5229$. These values reproduce Bishop's figure 1.17 well.

Kalman's output covariance P and RLS's output information Π represent uncertainty in the estimated coefficients. These do not directly yield uncertainties in the predicted labels, i.e., polynomials evaluated at each input point. For those, we follow Bishop's analysis and his equation 1.71.

In[82]:=
```
Manipulate[Module[{x},
```

```mathematica
With[{terms = symbolicPowers[x, M],
   cs = ϕ[M] /@ List /@ bts[[1]], ts = bts[[2]]},
  With[{normal = mleFit[M, bts],
    kalman = kalFit[10^(2 logσξ), 10^(2 logσξ)][M, bts]},
   With[{mleFn = terms.normal,
     kalFn = {terms}.kalman[[1]],
     bs2 = mapsSquared[10^(2 logσξ), 10^(2 logσξ), x, cs, M],
     mapFn = Quiet@mapMean[10^(2 logσξ), 10^(2 logσξ), x, cs, ts, M]},
    With[{lp = ListPlot[bts^T,
        PlotMarkers → {Graphics@{Blue, Circle[{0, 0}, 1]}, .05}]},
     Module[{showlist =
         {lp, Plot[Sin[2. π x], {x, 0., 1.}, PlotStyle → {Thick, Green}]}},
       If[mleQ, AppendTo[showlist, Plot[mleFn, {x, 0, 1},
          PlotStyle → {Orange}]]];
       If[kalQ, AppendTo[showlist,
         Plot[{kalFn, kalFn + √bs2 , kalFn - √bs2 }, {x, 0, 1},
          PlotStyle → {Cyan, {Thin, {Opacity[0], Cyan}},
             {Thin, {Opacity[0], Cyan}}}, Filling → {1 → {2}, 1 → {3}}]]];
       If[mapQ, AppendTo[showlist,
         Plot[{mapFn, mapFn + √bs2 , mapFn - √bs2 },
          {x, 0, 1},
          PlotStyle → {Magenta,
             {Thin, {Opacity[0], Magenta}}, {Thin, {Opacity[0], Magenta}}},
          Filling → {1 → {2}, 1 → {3}}]]];
       Quiet@Show[showlist, Frame → True, FrameLabel → {"x", "t"}]]]]]],
 Grid[{{Grid[{{Button["RESET", (M = 9;
          logσξ = Log10[√(1 / 0.09) ];
          logσξ = Log10[√0.005 ]) &],
       Control[{{kalQ, True, "KAL"}, {True, False}}],
       Control[{{mleQ, False, "MLE"}, {True, False}}],
       Control[{{mapQ, True, "MAP"}, {True, False}}]}}]},
   {Control[{{M, 9, "order M"}, 0, 16, 1, Appearance → {"Labeled"}}]},
   {Control[{{logσξ, Log10[√(1 / 0.09) ], "log σξ (KAL)"},
      -3, 5, Appearance → "Labeled"}]},
   {Control[{{logσξ, Log10[√0.005 ], "log σξ (KAL)"},
```

-5, 3, Appearance → "Labeled"}]}}]]

Out[82]=
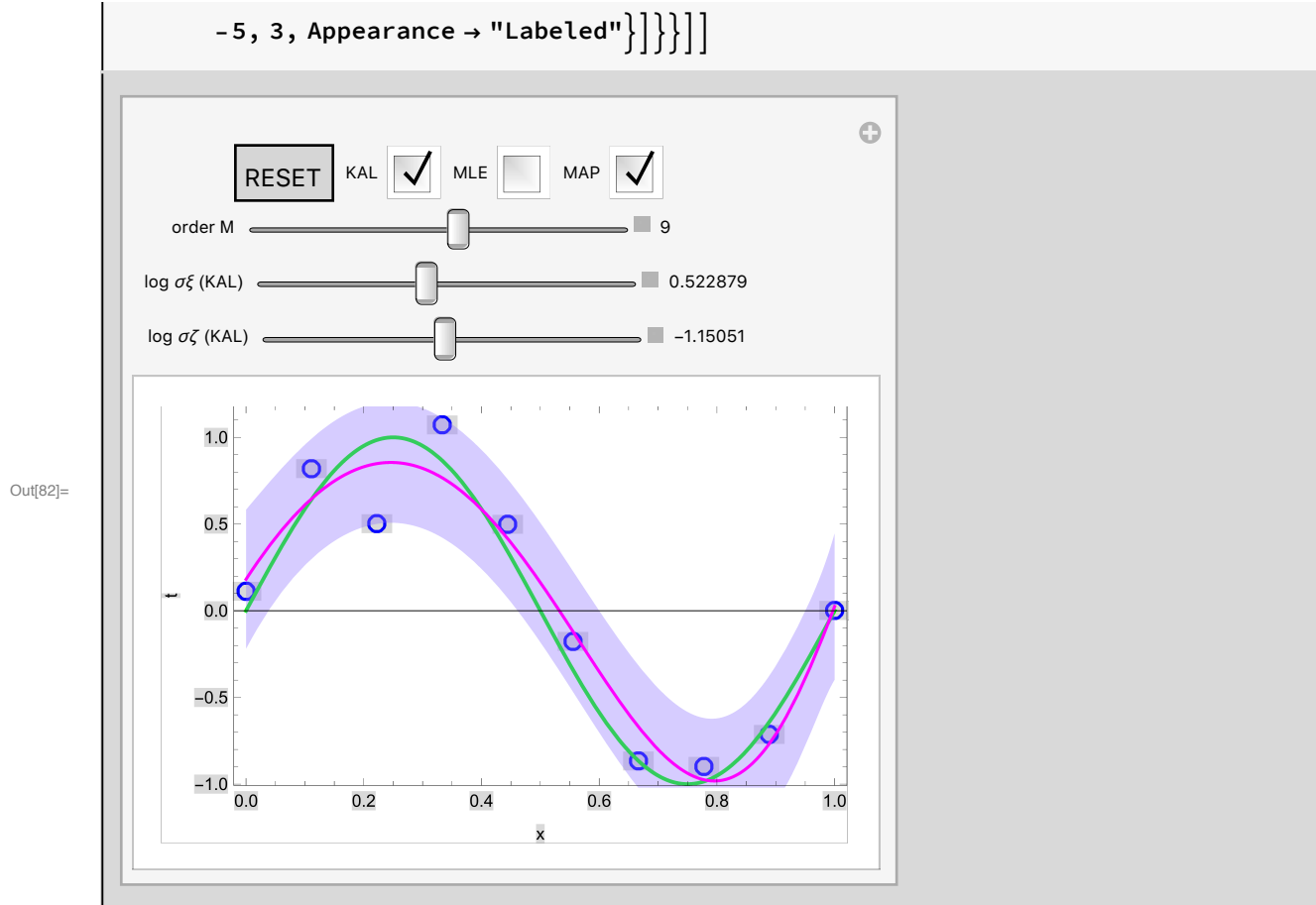
Conclusion

We have shown that Kalman folding (KAL) produces the same results as renormalized recurrent least squares (RLS) and maximum a-posteriori (MAP) for appropriate choices of covariances, i.e., regularization hyperparameters. We have further shown (numerically) that MAP produces the same results when its hyperparameters are swapped and inverted.

KAL and RLS offer significant advantages in space-time efficiency by avoiding storage and multiplication of large matrices. In all cases, we avoid matrix inverses by solving linear systems internally.