Efficient Bayesian Regularization

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December June 2023

Abstract

The contributions here are to:

- show numerical equivalence of three methods of linear regression: MAP (Maximum A-Posteriori), KAL (Kalman filtering/folding), and RLS (Recurrent Least Squares) when they are regularized by Bayesian a-priori beliefs, that is, protected from overfitting
- remove risky matrix inversion from MAP, KAL, and RLS
- remove expensive storage of observation vectors and matrices from MAP by rewriting MAP in recurrent form
- show numerical equivalence of KAL to recurrent MAP when MAP's regularization hyperparameters $\alpha = 1/\sigma_\xi^2$ and $\beta = 1/\sigma_\zeta^2$ are swapped and inverted
- conjecture formal equivalence and support the conjecture algebraically through order three
- sketch application of MAP, KAL, and RLS to Finite-Difference Policy Gradient in Reinforcement Learning
- apply all methods to a non-linear Padé approximant

Introduction

We investigate four popular methods for linear regression, i.e., parameter estimation, specifically with respect to the listed properties:

- MLE — Maximum Likelihood Estimation
  - Is exposed to overfitting.
  - Stores and inverts large matrices.
  - Has numerical hazards of matrix inversion.
- MAP — Maximum A-Posteriori
  - Addresses overfitting via regularization hyperparameters.
  - The standard algorithm stores and inverts large matrices.
  - When MAP's hyperparameters are swapped and inverted, MAP's recurrent form resembles KAL.

- KAL — Kalman filtering
  - Addresses overfitting via frank priors: estimates and covariances.
  - Runs in constant memory. The recurrent form is standard.
  - Dual co-Kalman and co-RLS address Finite-Difference Policy Gradient in Reinforcement Learning.
- RLS — Recurrent Least Squares
  - Matches KAL when renormalized by observation covariance.
  - Has apparently lower numerical risk than KAL.
  - Avoids subtraction in the covariance update.

We show that recurrent MAP, KAL, and RLS are numerically equivalent for appropriate choices of a-priori covariances. We conjecture that they're mathematically equivalent and present analytical evidence for the conjecture.

We note in passing that KAL and RLS admit full covariance (information) matrices, whilst MAP admits only standard deviations. MAP thus assumes that parameters and observations are non-dimensional and commensurate in scale. This means that practical application of MAP may require extra preconditioning steps. We do not dwell on this point in this article.

We show how to apply MAP, KAL, and RLS to an important practical problem: Finite-Difference Policy Gradient in Reinforcement Learning.

We close with a new example: Padé approximants. Linearization opens them to KAL and RLS filtering.

Overfitting and Regularization

Over-fitting is a hazard of linear regression. Linear models, as their number of parameters nears or exceeds the number of data points, follow the data too well — "wiggle too much." Such wiggling limits the utility of predictions. Between data points and outside data ranges, predictions become unreliable. We show visual demonstrations below after setting things up.

Regularization is the usual fix for over-fitting. Bayesian MAP regularizes via a-priori *belief hyperparameters* $\alpha = 1/\sigma_\xi^2$ and $\beta = 1/\sigma_\zeta^2$ — reciprocal variances of the unknown parameters ξ and the noise on observations ζ. MAP does not include prior estimates for the parameters ξ themselves.

Kalman filtering (KAL) and recurrent least squares (RLS) are structurally superior because they incorporate priors as extra observations with covariances. KAL and RLS can be stopped and restarted at any point in an infinite stream of observations, and do not need tuning.

RLS, renormalized with observation covariance, reproduces KAL and MAP within numerical errors. Renormalized RLS can have better numerical stability than KAL, trading off risk of ill-conditioning against risk of catastrophic cancelation.

We show below, algebraically through order three and numerically for orders higher than that, that MAP produces the same estimates as do KAL and renormalized RLS when α and β are swapped and inverted. After swapping and inverting α and β, the MAP equations resemble the equations of Kalman filtering, at least for the estimate. In post-processing, we un-swap and re-invert α and β to recover covariances from recurrent MAP.

MAP, KAL, and RLS all regularize, just in different ways.

KAL and RLS scale better than non-recurrent, full-storage MAP, which is a Bayesian modification of non-recurrent, full-storage MLE. There is no obvious way to convert MLE and MAP into recurrences, let alone to extend them to lazy sequences or asynchronous streams. KAL and RLS, however, are overtly recurrent. They are *foldable*: independent of the manner and means of data delivery. They avoid matrix storage, inversions, and multiplication.

Motivating Example

We begin with MLE a familiar school example: estimate the slope m and intercept b of the best-fit line function $z(x) = m\,x + b$ to noisy data $(x_i,\, z_i)$.

Think of $z(x) = m\,x + b$, more generally; as a linear combination of potentially non-linear *basis functions* of x with coefficients m and b. In the expression $z(x) = m\,x + b$, there are two basis functions. The first is $z_m(x) = x$, the identity function of x. The linear combination $m\,z_m(x) = m\,x$ happens, accidentally, to be linear in the independent variable x. Do not be distracted by that linearity; it is not the linearity we're looking for. The linearity of $m\,z_m(x) = m\,x$ in the parameter m is the interesting linearity. The second basis function, $z_b(x) = 1$, is the constant 1, non-linear in x. The linear combination $b\,z_b(x) = b \times 1 = b$ is linear in the parameter b. Thus the entire linear combination $z(x) = m\,z_m(x) + b\,z_b(x) = m\,x + b$ is linear in m and b, and all methods of estimating m and b are called *linear regression*.

The idea of linear combinations of non-linear functions extends to sophisticated models. A Fourier series $\sum_{k=0}^{\infty} a_k\, e^{i\,\omega_k\,x}$ is linear in the amplitudes a_k, but non-linear in the basis functions $e^{i\,\omega_k\,x}$. A linear combination of non-linear Bessel's functions approximates a vibrating drumhead. A linear combination of non-linear spherical harmonics approximates a lumpy Earth or a Hydrogen atom. These examples emphasize that linear regression methods like MLE, MAP, KAL, and RLS pertain to sophisticated models, linear in the parameters but non-linear in the independent variables.

MLE, Four Ways

We show numerical equivalence of four ways to do MLE:

1. (WBI) with Wolfram's built-in functions
2. (CNE) directly through the *classic normal equations*
3. (LPI) via the Moore-Penrose left pseudoinverse

4. (SLS) sidestepping the (hazardous?) inverse by solving a linear system

Problem Statement

Find best-fitting parameters m (slope) and b (intercept), where $z(x) = m\,x + b$, given known, noisy data $(z_1, z_2, \ldots, z_k)$ and abscissae $(x_1, x_2, \ldots, x_k)$. *Best-fitting* means *minimizing mean squared error*.

Write this *system* as a matrix equation:

- Z (*observations*; known, concrete, numerical; scalars in this example, but generalizable to vectors)
- A (*partials*, *Jacobian* of the observation model $z(x) = m\,x + b$ with respect to the unknown parameters $\Xi = (m, b)^\intercal$; rows containing values of basis functions $(x_{i\in[1..k]}, 1)$; known, concrete, numerical)
- $\Xi = (m, b)^\intercal$ (*model*, *aka state;* unknown *abstract, symbolic parameters* to be estimated).

N rows of data Z and N rows of partials A come in matched pairs.

$$Z_{N\times 1} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{pmatrix} = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{pmatrix} \cdot \begin{pmatrix} m_{\text{unknown}} \\ b_{\text{unknown}} \end{pmatrix} + \text{noise} \overset{\text{def}}{=} A_{N\times 2} \cdot \Xi_{2\times 1} + \text{samples of NormalDistribution}[0, \sigma_Z] \tag{1}$$

Ground Truth

Fake some data by (1) sampling a line specified by *ground truth* m_{GT} and b_{GT}, then (2) adding Gaussian observation noise. Run the faked data through the four estimation procedures WBI, CNE, LPI, SLS, and see how close the estimated $m_{\text{estimated}}$ and $b_{\text{estimated}}$ come to ground truth. This model is of order $M = 2$. There are $N = 119$ observed scalar data. Z is a column vector of dimension 119, a number picked arbitrarily.

In real-world applications, we rarely have ground truth. Its purpose here is to calibrate the four estimation procedures WBI, CNE, LPI, SLS.

Note and remember the ground-truth values $m_{\text{GT}} = 0.5$, $b_{\text{GT}} = -1/3$.

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

Partials

The partials inhabit an $N \times M$ matrix A, an order-N column vector of order-M row-co-vectors. Each co-vector is the Jacobian gradient 1-form of $A \cdot \Xi$ with respect to Ξ, the vector of unknown parameters, evaluated at specific values of Ξ from the data. Leave `partials` as a global variable for the following demonstrations.

- A major defect of MLE is that *A* and *Z* are large, potentially infinite, in row count. This defect is solved by recurrence, a major theme of this article.

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.},
 ≪113≫, {2.9322, 1.}, {2.9661, 1.}, {3., 1.}}
```

Faked Observations Z

Define a faking function and a global variable, `data`, for later use. Assume that the observations have unbiased (zero-mean) Gaussian white noise with variance $\sigma_Z = 0.65$, a convenient but arbitrary value.

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=

```
{0.398543, -0.334902, -0.261999, ≪113≫, 1.49818, 0.568748, 0.818659}
```

Wolfram Built-In

The Wolfram built-in `LinearModelFit` computes an MLE for $\Xi = \begin{pmatrix} m \\ b \end{pmatrix}$. The results in the cell below should approximate ground truth reasonably well (the results are randomized every time the notebook is evaluated).

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

```
Out[16]=
-0.277532 + 0.503776 x
```

Here is everything Wolfram has to say about this MLE (it’s a lot; use the notebook’s interactive buttons to expand and contract the display).

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

```
Out[17]=
⟨|AdjustedRSquared → 0.4387, AIC → 243.811, … 61 …, VarianceInflationFactors → {0., 1.}|⟩
Size in memory: 184.9 kB    + Show more    Show all    Iconize ▾
                            Store full expression in notebook
```

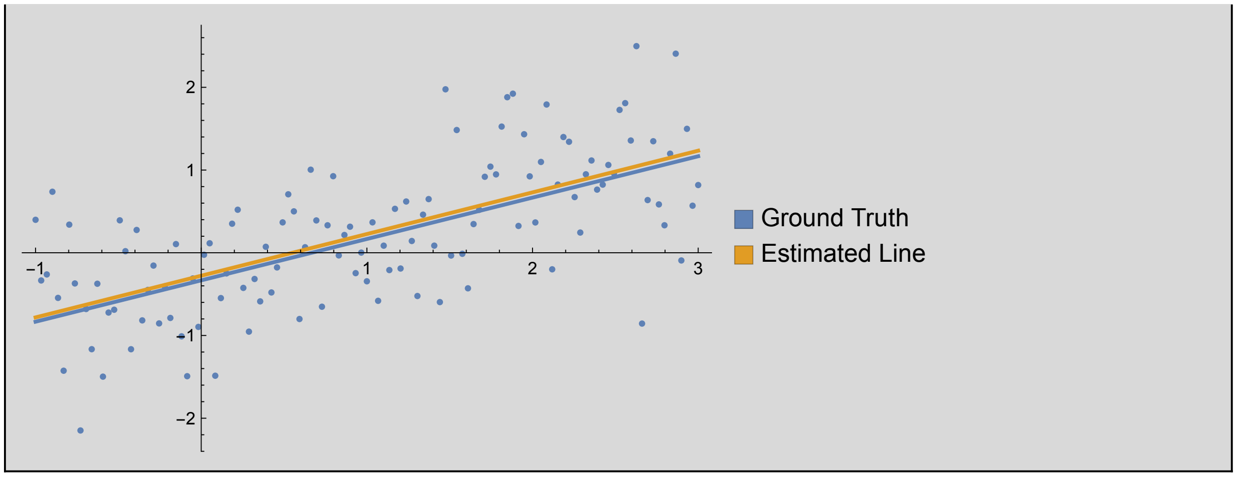
The most important attribute of the model is its covariance matrix. We come back to it below.

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

```
Out[18]//MatrixForm=
( 0.00641358  -0.00272231 )
( -0.00272231  0.00272231 )
```

The following plot shows that Wolfram does a god job of estimating the parameters *m* and *b*. We have 119 data and two parameters to estimate, so overfitting is not because the number of data greatly exceeds the number of parameters. We’ll show overfitting soon enough.

In[19]:=
```
Show[ListPlot[{partials⟦All, 1⟧, data}ᵀ],
 Plot[{m x + b, model[x]}, {x, min, max},
  PlotLegends → SwatchLegend[{"Ground Truth", "Estimated Line"}]]]
```
Out[19]=



Normal Equations

Solve Equation 1 for a concrete value of Ξ that minimizes sum-squared error $J(\Xi) \overset{\text{def}}{=} (Z - A\cdot\Xi)^{\mathsf{T}}\cdot(Z - A\cdot\Xi)$ of the *residuals* $(Z - A\cdot\Xi)$. That is the same as maximizing the likelihood $p(Z \mid \Xi)$ of the data Z given parameter values Ξ, giving MLE its name. Because the noise $\mathcal{N}(0, \sigma)$ is unbiased, the solution is exactly what one gets 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, just in the opposite order:

In[20]:=
```
Inverse[partialsᵀ.partials].partialsᵀ.data
model["BestFitParameters"]
```
Out[20]=
```
{0.503776, -0.277532}
```
Out[21]=
```
{-0.277532, 0.503776}
```

Moore-Penrose Left 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[22]:=
```
PseudoInverse[partials].data
```
Out[22]=
```
{0.503776, -0.277532}
```

Avoiding `Inverse`

In general, we advise replacing any occurrence of `Inverse[A].B` with `LinearSolve[A,B]`. See https://www.johndcook.com/blog/2010/01/19/dont-invert-that-matrix/.

In[23]:=
```
LinearSolve[partialsᵀ.partials, partialsᵀ].data
```
Out[23]=
```
{0.503776, -0.277532}
```

Do Not Use the Normal Equations

$(A^\intercal \cdot A)^{-1} \cdot A^\intercal \cdot Z$ is a nasty computation: big matrices, slow matrix multiplication, slow and numerically risky matrix inversion. How to avoid these hazards? Find a recurrence relation.

Recurrence

Recurrent Least Squares (RLS)

Derive, illustrate, and check a recurrent form of MLE. Regularize it (avoid overfitting) via Bayesian priors.

Fold the following recurrence over Z and A:

$$\begin{aligned} \xi &\leftarrow (\Lambda + [a^\intercal \cdot a])^{-1} \cdot ([a^\intercal \cdot \zeta] + [\Lambda \cdot \xi]) \\ \Lambda &\leftarrow (\Lambda + [a^\intercal \cdot a]) \end{aligned} \tag{3}$$

where

- ξ is the current estimate of Ξ, with prior ξ_0 for bootstrapping.
- a and ζ are matched, concrete, numerical rows of partials A and observations Z, as in Equation 1.
- Λ, with prior Λ_0, accumulates $A^\intercal \cdot A$ and implies the covariance matrix.

The priors ξ_0 and Λ_0 are the key to Bayesian regularization of RLS, as we shall see.

Derivation Sketch

Derive the recurrence as follows: Treat the estimate-so-far, including the Bayesian prior ξ_0 as its first observation:

$$\xi_{\text{so-far}} \overset{\text{def}}{=} (A_{\text{so-far}}{}^{\mathsf{T}} \cdot A_{\text{so-far}})^{-1} \cdot A_{\text{so-far}}{}^{\mathsf{T}} \cdot Z_{\text{so-far}} \tag{4}$$

Let Λ, the *information matrix*, be:

$$\Lambda = A_{\text{so-far}}{}^{\mathsf{T}} \cdot A_{\text{so-far}} \tag{5}$$

with its prior, Λ_0.

The scalar *performance* or *squared error* of the known estimate, $\xi_{\text{so-far}}$, is

$$J(\xi) \;=\; (Z_{\text{so-far}} - A_{\text{so-far}} \cdot \xi)^{\mathsf{T}} \cdot (Z_{\text{so-far}} - A_{\text{so-far}} \cdot \xi) \;=\; (\xi - \xi_{\text{so-far}})^{\mathsf{T}} \cdot \Lambda \cdot (\xi - \xi_{\text{so-far}}) \tag{6}$$

where

ξ is the unknown true parameter vector

$Z_{\text{so-far}}$ is the known, concrete column vector of all observations so-far

Equation 6 obtains because Λ is symmetric and because $\Lambda\, \xi_{\text{so-far}} = A_{\text{so-far}}\, Z_{\text{so-far}}$, from Equations 4 and 5.

Adding a new observation, ζ, and its corresponding partial row co-vector 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 the unknown ξ to find the recurrence (set the derivative of J with respect to ξ to zero and solve the resulting system). ■

RLS introduces an a-priori estimate ξ_0 and an a-priori information matrix Λ_0. RLS is therefore Bayesian by construction. When *renormalized* with an a-priori covariance for the observations ζ, the recurrence relation in Equation 3 is equivalent to KAL and numerically equivalent to MAP. We show the renormalization procedure in a later section. Rigorous proof of equivalence to MAP for all orders awaits future work, though *Mathematica* can prove it through order 3.

Numerical Demonstration

Bootstrap the recurrence with ad-hoc, a-priori values $\xi_0 = (\,0 \;\; 0\,)^{\mathsf{T}}$ and $\Lambda_0 = ((\,10^{-6} \;\; 0\,)\,(\,0 \;\; 10^{-6}\,))$ — not much but just enough prior information. `Update` is *foldable* RLS. Avoid `Inverse` via `LinearSolve`.

In[24]:=
```
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,
    (* priors *)
    {(0
      0), (1.0*^-6    0
           0      1.0*^-6)},
    (* sequence of observations and partials *)
    {List /@ data, List /@ partials}ᵀ])
```

Out[26]=
```
{( 0.503776 ), (280.356  119.)}
 (-0.277532)   ( 119.    119.)
```

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 has negligible effect.

Structural Notes

The highlighted mappings of `List` over the data and partials lists convert them from 1-dimensional puns of column vectors into 2-D column vectors.

Memory and Time Efficiency

Because the observations and partial are the third argument of Fold, they need not be stored. They might as well be infinite and / or asynchronous streams. See https://community.wolfram.com/-groups/-/m/t/3078712 and https://community.wolfram.com/groups/-/m/t/3074231.

The required memory for RLS is $O(M^2)$, where M is the order of the model = the number of parameters to estimate = the length of Ξ = the length of each row of A, almost always small enough to fit in memory. The recurrence does not depend on the number N of data items.

RLS consumes $O(M^3)$ time for `LinearSolve` at each step of the recurrence .

Contrast with the normal equations, which require $O(N\,M)$ storage for A and Z and $O(N\,M)$ time for $A^{\intercal}.Z$. N can be much larger than M or even M^2. N can even be infinite, making the normal equations impossible.

Check the a-priori

The final value of Λ (called Π, a returned value), is $A_{\text{full}}^{\mathsf{T}} \cdot A_{\text{full}} + \Lambda_0$. Check that the difference between Π and $A_{\text{full}}^{\mathsf{T}} \cdot A_{\text{full}}$ equals Λ_0, the a-priori covariance.

```
In[27]:=  Π - partialsᵀ.partials
Out[27]=
{{1. × 10^-6, 0.}, {0., 1. × 10^-6}}
```

Covariance of the Estimate

The covariance of this estimate Ξ is $\left(\frac{n-1}{n-2}\right) *$Variance[Z – $A \cdot$Ξ] 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 is the number of parameters estimated, the *degrees of freedom* (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). In general, the denominator of the correction is $n - p$, where n is the number of data and p is the number of parameters being estimated.

```
In[28]:=  Inverse[partialsᵀ.partials] * (nData - 1)/(nData - 2) *
            Variance[data - partials.{mBar, bBar}] // MatrixForm
Out[28]//MatrixForm=
 ( 0.00272231  -0.00272231 )
 (-0.00272231   0.00641358 )
```

Check that this covariance approximately equals that deduced from Π, the final value of Λ:

```
In[29]:=  (cov$ = Inverse[Π] * (nData - 1)/(nData - 2) * Variance[data - partials.{mBar, bBar}]) //
           MatrixForm
Out[29]//MatrixForm=
 ( 0.00272231  -0.00272231 )
 (-0.00272231   0.00641358 )
```

This is the same covariance matrix that Wolfram’s **`LinearModel`** reports. This second check of our recurrence succeeds.

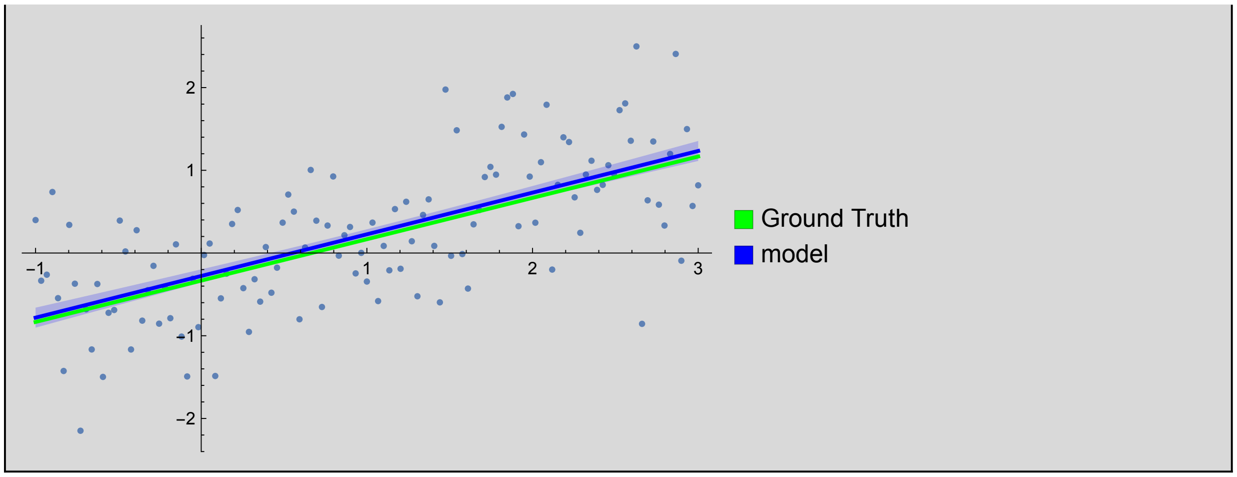
```
In[30]:=  Reverse@(Reverse /@ model["CovarianceMatrix"]) // MatrixForm
Out[30]//MatrixForm=
 ( 0.00272231  -0.00272231 )
 (-0.00272231   0.00641358 )
```

Covariance of the Prediction

If we view the two parameters, *m* and *b*, as random variables, then the predicted value *z* at every input point *x* is a linear combination of random variables, thus a random variable. The following plot shows the one-sigma band around the predicted values.

In[31]:=
```
Module[{row, diagonalTerm, offDiagonalTerm, Σ},
 row[x_] := {{x, 1.}};
 diagonalTerm[x_] := Map[Dot[Diagonal[cov$], #] &, #^2 & /@ row[x]];
 offDiagonalTerm[x_] := MapThread[Dot, {row[x].cov$, row[x]}];
 Σ[x_] := Sqrt[(row[x].cov$.row[x]ᵀ)⟦1, 1⟧];
 With[{points = {partials⟦All, 1⟧, data}ᵀ},
  Show[ListPlot[{points}],
   Plot[{m x + b,
     model[x],
     model[x] + Σ[x],
     model[x] - Σ[x]}, {x, min, max},
    PlotStyle → {
      Green, Blue,
      {Thin, {Opacity[0], Blue}},
      {Thin, {Opacity[0], Blue}}},
    Filling → {2 → {3}, 2 → {4}},
    PlotLegends → SwatchLegend[{"Ground Truth", "model"}]]]]]
```

Out[31]=



Interim Conclusions

We have (notionally) eliminated $O(N M)$ memory bloat by processing updates one observation at a time, each with its paired partial. When N exceeds memory or is infinite, this elimination is essential. The resulting forms are $O(M)$ in storage, where M is the order of the model, almost always small enough to store in memory. The JPL Horizon project has a model with some 1.5 million parameters, for instance, still easy to fit in memory.

We reduce numerical risk by solving a linear system instead of inverting a matrix.

We avoid multiplication of $O(N\,M)$ matrices, which may infeasible.

We still have work to do with renormalization and observation covariances.

Regularization and Renormalization

Chris Bishop's *Pattern Recognition and Machine Learning* has an extended example of fitting polynomials 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. KAL and RLS regularize by construction. In this section, we relate KAL and RLS regularization by frank priors to Bishop's MAP regularization by hyperparameters.

To bootstrap recurrences, KAL and RLS require a-priori estimates of the unknown parameters and their uncertainties. RLS takes the a-priori uncertainty of parameters as an information matrix; KAL takes it as a covariance matrix, inverse of the information matrix. Bishop also computes the information matrix as S^{-1}, though he does not name it so. KAL additionally requires an a-priori estimate of observation noise. We show how to *renormalize* RLS with observation noise to produce results equivalent to KAL and MAP.

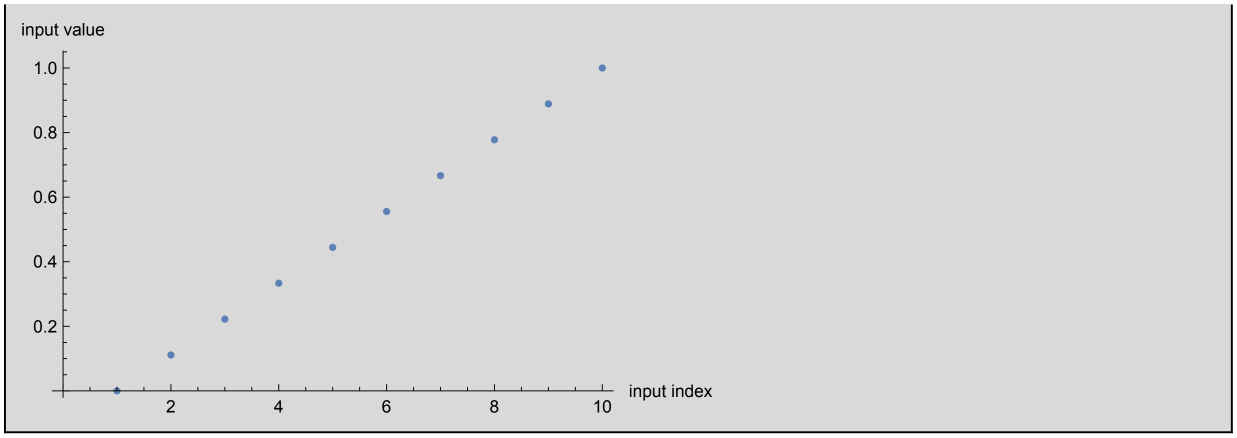
Reproducing Bishop's Example

Bishop's Training Set

First, create a sequence of $N = 10$ inputs, equally spaced in $[0, 1]$.

In[32]:=
```
ClearAll[bishopTrainingSetX];
bishopTrainingSetX[N_] := Array[Identity, N, {0., 1.}];
ListPlot[bishopTrainingSetX[10], AxesLabel → {"input index", "input value"}]
```

Out[34]=



Bishop’s ground truth is a single cycle of a sine wave. Add noise to a sample of that ground truth taken at the inputs above. Bishop doesn’t state his observation noise, but I’ve reverse engineered $\sigma_z = \sigma_t = 0.30$ 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. Bishop’s notation for normal distribution takes variance as second argument, so beware.

In[35]:=
```
ClearAll[bishopTrainingSetY, bishopGroundTruthY];
bishopGroundTruthY[xs_] := Sin[2. π #] & /@ xs;
bishopTrainingSetY[xs_, σ_] :=
  With[{n = Length@xs},
   bishopGroundTruthY[xs]
    + RandomVariate[NormalDistribution[0., σ], n]];
```

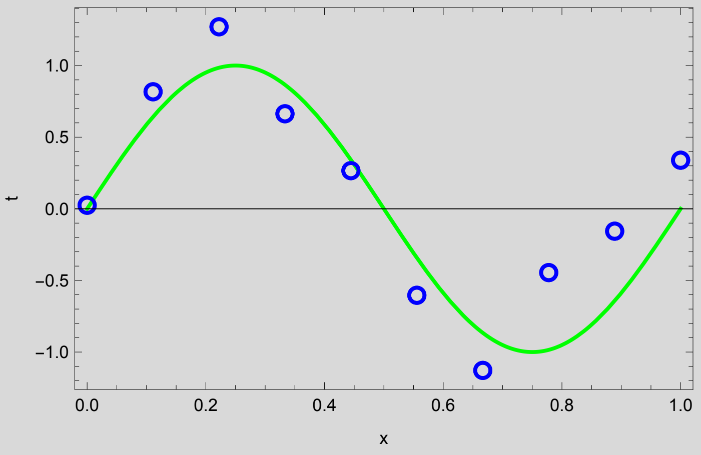
Take a sample of the outputs and assign it the name `bts` for `bishopTrainingSet`. It is not his actual training set, which I did not find in print, just my simulation.

In[38]:=
```
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[42]:=
```
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[42]=



Partials: Gradients of the Unknown Parameters

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

In[43]:=
```
ClearAll[partialsFn];
partialsFn[order_, xs_] :=
  Transpose@Quiet@Table[#^(i-1) /. {Indeterminate → 1}, {i, order + 1}] &@xs;
MatrixForm@partialsFn[6, {x₁, x₂, x_M}]
```

Out[45]//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 Observation Equations

Confer Bishop’s Equation 3.3, page 138. He writes the parameters-to-estimate as $\boldsymbol{w}$ and he writes the observation equation as

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

(*bias* is the coefficient w_0 of the 0th basis function). This is predictive: you give me concrete inputs $\boldsymbol{x}$ and parameters $\boldsymbol{w}$, and I’ll give you a predicted observation y in terms of the M + 1 basis functions $\boldsymbol{\phi}$

corresponding to the $M+1$ unknown parameters $\boldsymbol{w}$. The basis functions need not be polynomials. They can be anything: wavelets, Fourier waves, Chebyshev polynomials, etc.

Bishop transposes $\boldsymbol{w}$ into a co-vector and writes

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

where $\boldsymbol{\phi}(\boldsymbol{x})$ is an $(M+1)$-dimensional column-vector of basis functions, each a transpose of one row of our partials matrix A. We prefer always to think of partials or gradients as co-vectors. See https://en.wikipedia.org/wiki/Covariance_and_contravariance _of _vectors, https://math.stackexchange.com/questions/1172022, and https://math.stackexchange.com/questions/54355).

To find best-fit values for $\boldsymbol{w}$, rows of the partials matrix A are the co-vector gradients of y with respect to $\boldsymbol{w}$. We prefer to write

- *observations* as height-N column-vector Z_{N} with elements $\zeta_{j\in[1..\mathrm{N}]}$
- the *model* or unknown parameters, an $(M+1)$-dimensional column-vector $\Xi_{(M+1)\times 1}$ with elements $\xi_{i\in[0..M]}$ (here, ξ_0 is not a vector prior, but a bias term)
- *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 $\boldsymbol{x}_{n\in[1..N]}$. Bishop works in the dual of our formulation, that is, already set up for finite-difference policy-gradient estimation.

Our KAL and RLS express co-vector rows of the design matrix as polynomial basis functions evaluated at the input points $x_{n\in[1..\mathrm{N}]}$:

$$Z \;=\; A\cdot\Xi \;=\; \begin{pmatrix}\zeta_0\\ \zeta_1\\ \vdots\\ \zeta_{\mathrm{N}}\end{pmatrix} \;=\; \begin{pmatrix}1=x_1^0 & x_1 & x_1^2 & \cdots & x_1^M\\ 1=x_2^0 & x_2 & x_2^2 & \cdots & x_2^M\\ \vdots & \vdots & & \ddots & \vdots\\ 1=x_N^0 & x_N & x_N^2 & \cdots & x_N^M\end{pmatrix}\cdot\begin{pmatrix}\xi_0\\ \xi_1\\ \vdots\\ \xi_{\mathrm{M}}\end{pmatrix} + \text{noise} \tag{7}$$

then packed up into rows of the A matrix.

$$Z \;=\; A\cdot\Xi \;=\; \begin{pmatrix}\zeta_0\\ \zeta_1\\ \vdots\\ \zeta_{\mathrm{N}}\end{pmatrix} \;=\; \begin{pmatrix}A_{1\times(\mathrm{M}+1)}\,(x_1)\\ A_{1\times(\mathrm{M}+1)}\,(x_2)\\ \vdots\\ A_{1\times(\mathrm{M}+1)}\,(x_{\mathrm{N}})\end{pmatrix}_{\mathrm{N}\times(\mathrm{M}+1)}\cdot\begin{pmatrix}\xi_0\\ \xi_1\\ \vdots\\ \xi_{\mathrm{M}}\end{pmatrix} + \text{noise} \tag{8}$$

MLE: The Normal Equations

For comparison purposes, mechanize the normal equations. Expect them to over-fit.

In[46]:=

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

Out[48]=

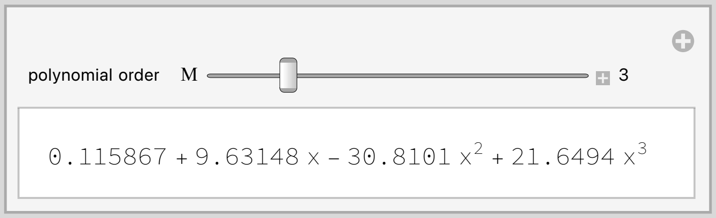
```
{0.115867, 9.63148, -30.8101, 21.6494}
```

The normal equations as a symbolic polynomial on **bts** follows. Notice we can increase the order beyond the number of data, creating an underdetermined system. Underdetermined systems are not typical in real-world data processing. Usually the number of data exceed the order and the system is overdetermined. The pseudoinverse in *mleFit* is agnostic to the distinction.

In[49]:=

```
ClearAll[symbolicPowers];
symbolicPowers[variable_, order_] :=
  partialsFn[order, {variable}]⟦1⟧;
ClearAll[x];
Manipulate[
 symbolicPowers[x, M].mleFit[M, bts],
 {{M, 3, "polynomial order M"}, 0, 16, 1, Appearance → {"Labeled"}}]
```

Out[52]=



polynomial order M 3

```
0.115867 + 9.63148 x - 30.8101 x^2 + 21.6494 x^3
```

RLS: Recurrent Least Squares

Regularize RLS by its a-priori estimate of the unknown parameters and by its a-priori information matrix. Slide the slider in the display below to decrease the incoming σ^2 of the information matrix by orders of magnitude. Check that, once the info becomes too small, the Λ matrix becomes ill-conditioned: pink warning message appear from the Wolfram kernel, and the solution becomes numerically suspect. In the rest of this article, we eliminate these error message by applying Wolfram's **Quiet** because we notice, empirically, that ill-conditioning of the information matrix does not seem harmful for this example. However, ill-conditioning is a problem in practice and must be tracked and managed with methods out-of-scope in this article.

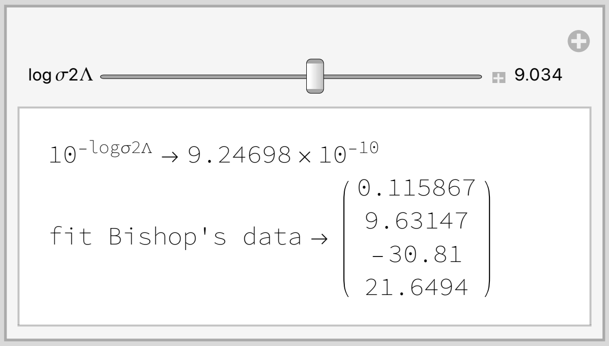
Non-Renormalized RLS Fitting Procedure

In[53]:=

```
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[
 Column[{"10^-logσ2Λ" → 10^-logσ2Λ,
   "fit Bishop's data" → (rlsFit[10^-logσ2Λ][3, bts]⟦1⟧ // MatrixForm)}],
 {{logσ2Λ, 9.034}, 0, 16, Appearance → "Labeled"}]
```

Out[55]=



```
log σ2Λ  9.034

10^-logσ2Λ → 9.24698 × 10^-10

fit Bishop's data → ( 0.115867
                      9.63147
                      -30.81
                      21.6494 )
```

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 therefore 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 is why we *lambda-lift* P_Z into its own function slot. **`kalmanUpdate`**, given some concrete value of $P_Z = \sigma_\zeta^2\, \mathcal{I}$, yields a foldable function of {current state, covariance} and of {new data, partials}. Initialize the fold in **`kalFit`** with a-priori estimate $\xi_0 = 0$ and covariance $P_0 = \sigma_\xi^2\, \mathcal{I}$, and run the fold over observation-and-partial pairs $\{\zeta, a\}$.

Kalman Fitting Procedure

In[56]:=
```
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[σζ2_, σξ2_][order_, trainingSet_] :=
  With[{xs = trainingSet⟦1⟧, ys = trainingSet⟦2⟧},
   With[{ξ0 = List /@ ConstantArray[0, order + 1],
     P0 = σξ2 * IdentityMatrix[order + 1]},
    Fold[kalmanUpdate[σζ2 * IdentityMatrix[1]],
     {ξ0, P0},
     {List /@ ys, List /@ partialsFn[order, xs]}ᵀ]]];
```

See All Three

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

On a 9th-order polynomial, both KAL and RLS regularize when the a-priori information is $10^{-6}\,\mathcal{I}$ and the a-priori covariance is $10^{6}\,\mathcal{I}$. In contrast, the MLE over-fits a by running through every data point. A 9th-order polynomial fits the $M+1=10$ data points of the example exactly.

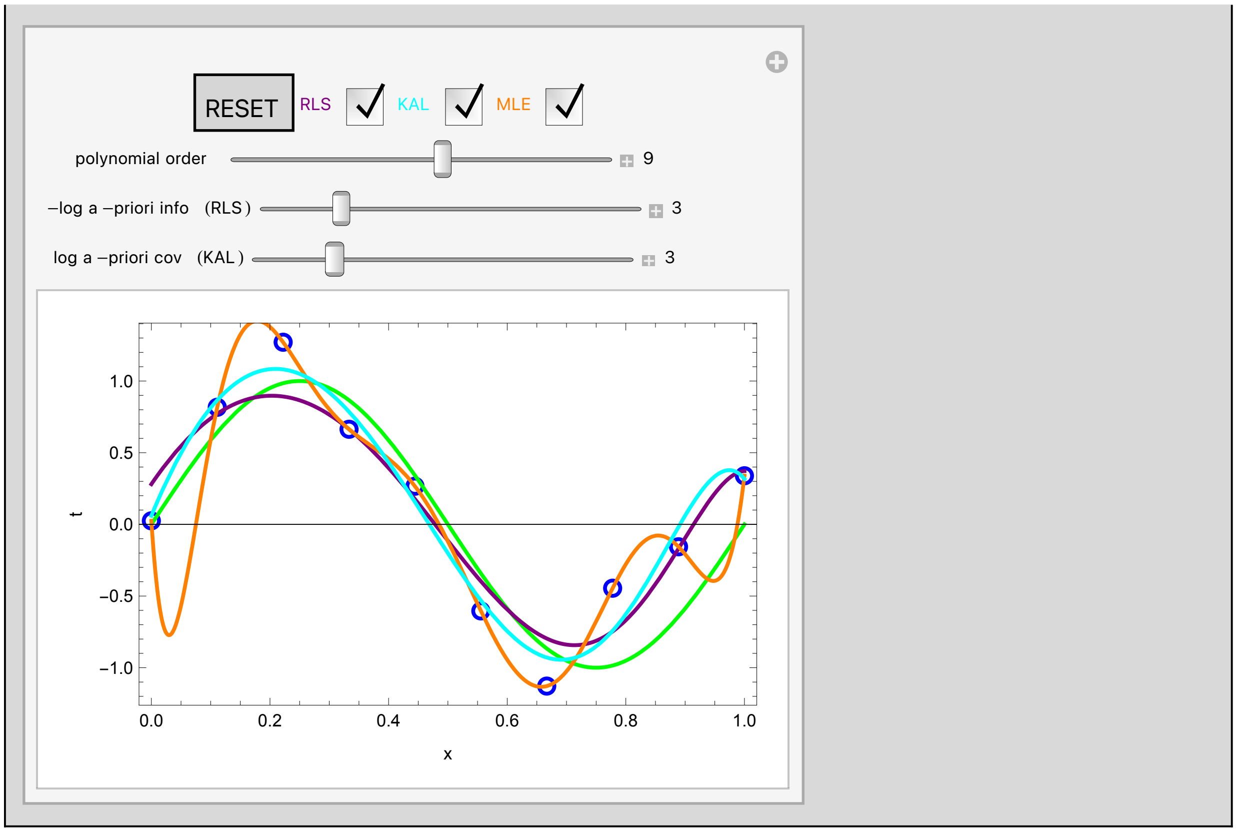
Increasing `-logΛ` *decreases* a-priori information in RLS, decreasing belief in the a-priori ξ_0. Increasing `logσξ2` *increases* the a-priori covariance $\sigma_{\xi_0}^2$ of ξ_0, also decreasing belief in ξ_0. As $\sigma_{\xi_0}^2$ increases, RLS and KAL eventually over-fit and align with MLE. Later, we show that MAP similarly over-fits as belief in ξ_0 decreases.

Run the polynomial order up to nine, then run `-logΛ` and `logσξ2` all the way to the right, to their maximum values, to see overfitting, that is, failure of regularization.

The **G**reen line is **G**round Truth.

In[59]:=
```
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, Style["RLS", Bold, Purple]}, {True, False}}],
       Control[{{kalQ, True, Style["KAL", Bold, Cyan]}, {True, False}}],
       Control[{{mleQ, True, Style["MLE", Bold, Orange]}, {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[59]=



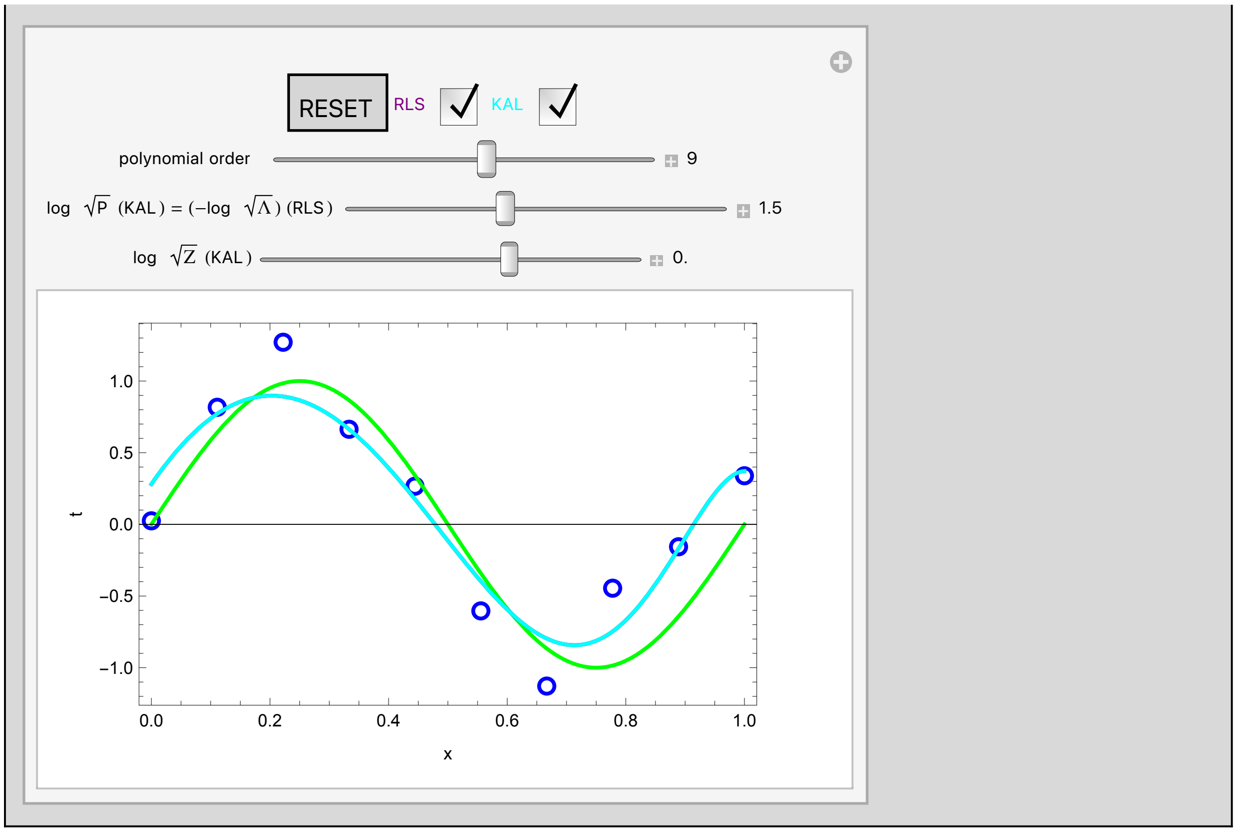
Renormalizing RLS

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 KAL's a-priori covariance *P*. KAL and RLS will have the same belief in the a-priori parameters ξ_0. Vary the observation noise independently to see KAL and RLS coincide when the observation noise is unity (its log is zero).

As observation noise decreases, the solutions believe the observations more than the a-prioris and RLS and KAL over-fit. As a-priori covariance decreases, RLS and KAL believe the a-prioris more than the observations and the solution regularizes.

In[60]:=
```
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, Style["RLS", Bold, Purple]}, {True, False}}],
       Control[{{kalQ, True, Style["KAL", Bold, Cyan]}, {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[60]=



Renormalized RLS

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

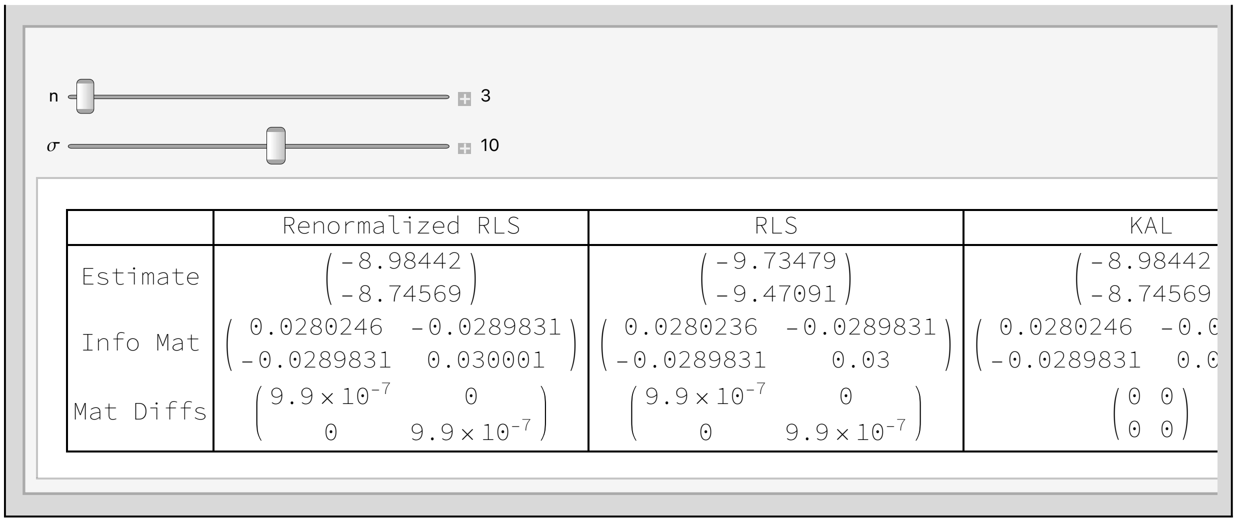
Scale (each row of) the partials by $1/\sigma_Z$ the inverse of the observation standard deviation σ_Z. Rescale the final estimate (not the final covariance) by a matrix built from $1/\sigma_Z$ because the recurrent normal equation, $\left(P_Z^{-1}\, A^\intercal\, A\, P_Z^{-T}\right)^{-1} P_Z^{-1}\, A^\intercal\, Z$, has one too many factors of P_Z.

Redefine `rlsUpdate` to include this renormalization and notice that it’s always equal to KAL.

In[61]:=
```
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
             0), Λ0 = (1.0*^-6    0
                         0     1.0*^-6), m = MatrixForm,
   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[σ^2], {ξ0, Inverse@Λ0}, inputs]);
   Grid[{
     {"", "Renormalized RLS", "RLS", "KAL"},
     {"Estimate", m[IdentityMatrix[2]/σ .ξrr], m@ξr, m@ξk},
     {"Info Mat", m@Πrr, m[Πr / σ^2], m[Inverse@Πk]},
     {"Mat Diffs",
      m@Chop[Abs[Πrr - Πr / σ^2], 10^-9],
      m@Chop[Abs[Inverse@Πk - Πr / σ^2], 10^-9],
      m@Chop[Abs[Inverse@Πk - Πrr], 10^-9]]}},
    Frame → {All, {True, True, None}}]]],
 {{n, 3}, 3, nData, 1, Appearance → "Labeled"},
 {{σ, 10}, -100, 100, Appearance → "Labeled"}]
```

Out[63]=



n 3

σ 10

	Renormalized RLS	RLS	KAL
Estimate	$\begin{pmatrix} -8.98442 \\ -8.74569 \end{pmatrix}$	$\begin{pmatrix} -9.73479 \\ -9.47091 \end{pmatrix}$	$\begin{pmatrix} -8.98442 \\ -8.74569 \end{pmatrix}$
Info Mat	$\begin{pmatrix} 0.0280246 & -0.0289831 \\ -0.0289831 & 0.030001 \end{pmatrix}$	$\begin{pmatrix} 0.0280236 & -0.0289831 \\ -0.0289831 & 0.03 \end{pmatrix}$	$\begin{pmatrix} 0.0280246 & -0.0 \\ -0.0289831 & 0.0 \end{pmatrix}$
Mat Diffs	$\begin{pmatrix} 9.9\times10^{-7} & 0 \\ 0 & 9.9\times10^{-7} \end{pmatrix}$	$\begin{pmatrix} 9.9\times10^{-7} & 0 \\ 0 & 9.9\times10^{-7} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

Renormalized RLS beats KAL

KAL and renormalized RLS are mathematically equivalent (stated withoutt proof). Operationally, KAL subtracts matrices to update estimated covariance. Subtraction is exposed to catastrophic cancelation. Renormalized RLS only adds to the information matrix, so is exposed only to ill-conditioning, which is empirically less severe than catastrophic cancelation. We show this below.

Regularization and MAP

Bishop reports $\beta = 11.111\ldots$ and $\alpha = 0.005$ in his figure 1.17 (page 32) and in his Equations 1.70 through 1.72 (page 31). These equations look suspiciously like the equations for Kalman filtering. Bishop's matrix $\boldsymbol{S}$ looks like $\boldsymbol{D}^{-1}$ in `kalmanUpdate` above. Let's reproduce MAP via KAL and renormalized RLS.

Bishop's MAP

The MAP Equations

Bishop's Equations 1.70 through 1.72 are reproduced here. The dimensions of the identity matrix in S are M + 1, where M is the order of the polynomial model, one more than M to account for a bias term. It turns out that Bishop's S^{-1} is exactly the information matrix of RLS, as we see in the section on *Covariance of the Prediction*, below. Bishop's hyperparameters, $\alpha = 1/\sigma_\xi^2$ and $\beta = 1/\sigma_\zeta^2$, are reciprocal variances of the a-priori estimates and the observations, respectively.

$$m(x) \;=\; \beta\,\phi(x)^{\mathsf{T}}\cdot S\cdot \sum_{n=1}^{N} \phi(x_n)\, t_n \tag{9}$$

$$s^2(x) \;=\; \beta^{-1} + \phi(x)^{\mathsf{T}} \cdot S \cdot \phi(x) \tag{10}$$

$$S^{-1} \overset{\text{def}}{=} \alpha\, I_{M+1} + \beta \sum_{n=1}^{N} \phi(x_n) \cdot \phi(x_n)^{\mathsf{T}} \tag{11}$$

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

$$\sum_{n=1}^{N} \phi(x_n)\, t_n = A^{\mathsf{T}} \cdot Z \tag{12}$$

$$\lim_{\alpha \to 0} \left(\beta^{-1} S^{-1}\right) = A^{\mathsf{T}} \cdot A \tag{13}$$

Φ Vectors

Bishop’s $\phi(x_n)$ is an $(M + 1)$-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 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 all the operational ills of the normal equations: too much memory, too much time, and numerical risk.

```
In[64]:= ClearAll[ϕ];
         ϕ[M_][xn_] := Quiet@Table[xn^i, {i, 0, M}] /. {Indeterminate → 1};
         MatrixForm /@ ϕ[3] /@ List /@ bts⟦1⟧
```

```
Out[66]=
{(1 ), (1.        ), (1.        ), (1.        ), (1.        ),
 (0.), (0.111111  ), (0.222222  ), (0.333333  ), (0.444444  ),
 (0.), (0.0123457 ), (0.0493827 ), (0.111111  ), (0.197531  ),
 (0.), (0.00137174), (0.0109739 ), (0.037037  ), (0.0877915 ),

 (1.      ), (1.      ), (1.      ), (1.      ), (1.)}
 (0.555556), (0.666667), (0.777778), (0.888889), (1.)
 (0.308642), (0.444444), (0.604938), (0.790123), (1.)
 (0.171468), (0.296296), (0.470508), (0.702332), (1.)
```

S Inverse

Bishop’s Equation 1.72.

```
In[67]:= 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, replacing `Inverse` with `LinearSolve` as we usually do:

```
In[69]:=
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 of the observations ζ. The predicted observation 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.

Mean Is Invariant Under “Swap and Invert”

We observe, numerically and algebraically through order 3, that Bishop's equations for the estimate match KAL and RLS when the covariances are swapped and inverted, that is, when β is σ_ξ^2 and when $\alpha = \sigma_\zeta^2$. The demonstration below shows symbolically that the estimates (not covariances) `m1≡ mapMean[α,β,x,cs,ts,M]` and `m2≡mapMean[1/β,1/α,x,cs,ts,M]`, are equal. *Mathematica* has trouble simplifying `m1-m2`, for orders 1 and 4. For order 1, visual inspection of m1 and m2 reveal approximate equality. For orders 4 and greater, we rely on the numerical check. For fun, we include symbolic forms for the information matrix, `sInv[α,β,cs,M]` and a nominal form `sInv[1/β,1/α,cs,M]`. We invite readers to perform rigorous analysis and even find a proof.

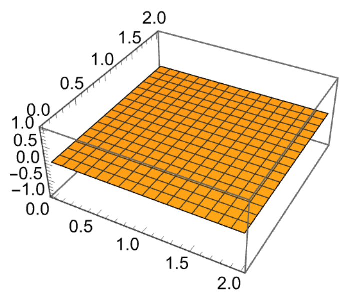
In[71]:=
```
ClearAll[x, α, β, chopQ];
DynamicModule[{chopQ = True},
 Manipulate[With[{cs = ϕ[M] /@ List /@ bts⟦1⟧, ts = bts⟦2⟧,
    pf = If[chopQ, Chop, Identity] @* FullSimplify},
   With[{m1 = mapMean[α, β, x, cs, ts, M],
     m2 = mapMean[1/β, 1/α, x, cs, ts, M]},
    Grid[(   "m1"                pf@m1
             "m2"                pf@m2
           "m1-m2"             pf[m1 - m2]
         "N(m1-m2)" Plot3D[Log10[1 + pf[m1 - m2]],
                       {α, 0, 2.0},
                       {β, 0, 2.0}]          ), Frame → All]]],
  Column[{Row[{Button["UN-CHOP", chopQ = False], "         ",
      Button["CHOP", chopQ = True]}],
    Control[{{M, 2, "order M"}, 0, 9, 1, Appearance → {"Open", "Labeled"}}]}]]]
```

Out[72]=

UN−CHOP CHOP

order M 2

2

m1	$\left(\beta\left((8.47776+(-4.21803-4.39019\,x)\,x)\,\alpha^7+(213.327+(-145.493-143.305\,x)\,x)\,\alpha^6\,\beta+(1368.31+(-1286.01-1187.\,x)\,x)\,\alpha^5\,\beta^2+(672.392+(-884.71-409.533\,x)\,x)\,\alpha^4\,\beta^3+(-1205.45+x\,(1060.66+1227.97\,x))\,\alpha^3\,\beta^4+(199.136+(-5.54472-419.131\,x)\,x)\,\alpha^2\,\beta^5+(31.8217+x\,(-71.0068+24.5802\,x))\,\alpha\,\beta^6+(0.864241+x\,(-2.68997+1.66404\,x))\,\beta^7\right)\right)/\left(2.84487\,\alpha^4+43.8868\,\alpha^3\,\beta+42.3378\,\alpha^2\,\beta^2-24.1205\,\alpha\,\beta^3-1.\,\beta^4\right)^2$
m2	$\left(\beta\left((-2.98002+x\,(1.48268+1.5432\,x))\,\alpha^3+(-29.0147+x\,(28.2694+26.5666\,x))\,\alpha^2\,\beta+(10.9758+(-6.1235-15.5571\,x)\,x)\,\alpha\,\beta^2+(0.864241+x\,(-2.68997+1.66404\,x))\,\beta^3\right)\right)/\left(-2.84487\,\alpha^4-43.8868\,\alpha^3\,\beta-42.3378\,\alpha^2\,\beta^2+24.1205\,\alpha\,\beta^3+1.\,\beta^4\right)$
m1−m2	0
N(m1−m2)	

Numerical Equivalences

In the following demonstration, the numerical evidence for equality of the estimates (not equality of the covariances) produced by 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 $M = 4$. For high σ_ξ^2 (we do not believe the a-priori estimate of ξ) or low σ_ζ^2 (we *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, $(I - K a) P$, becomes ill-conditioned, if not negative, because $K a$ is near the identity. Other articles in this series mitigate this defect via alternative, mathematically equivalent, forms for P.

RLS does not suffer from these ills because it never subtracts. RLS is still exposed to ill-conditioning of the information matrix, but that seems numerically less harmful to the final result in this example.

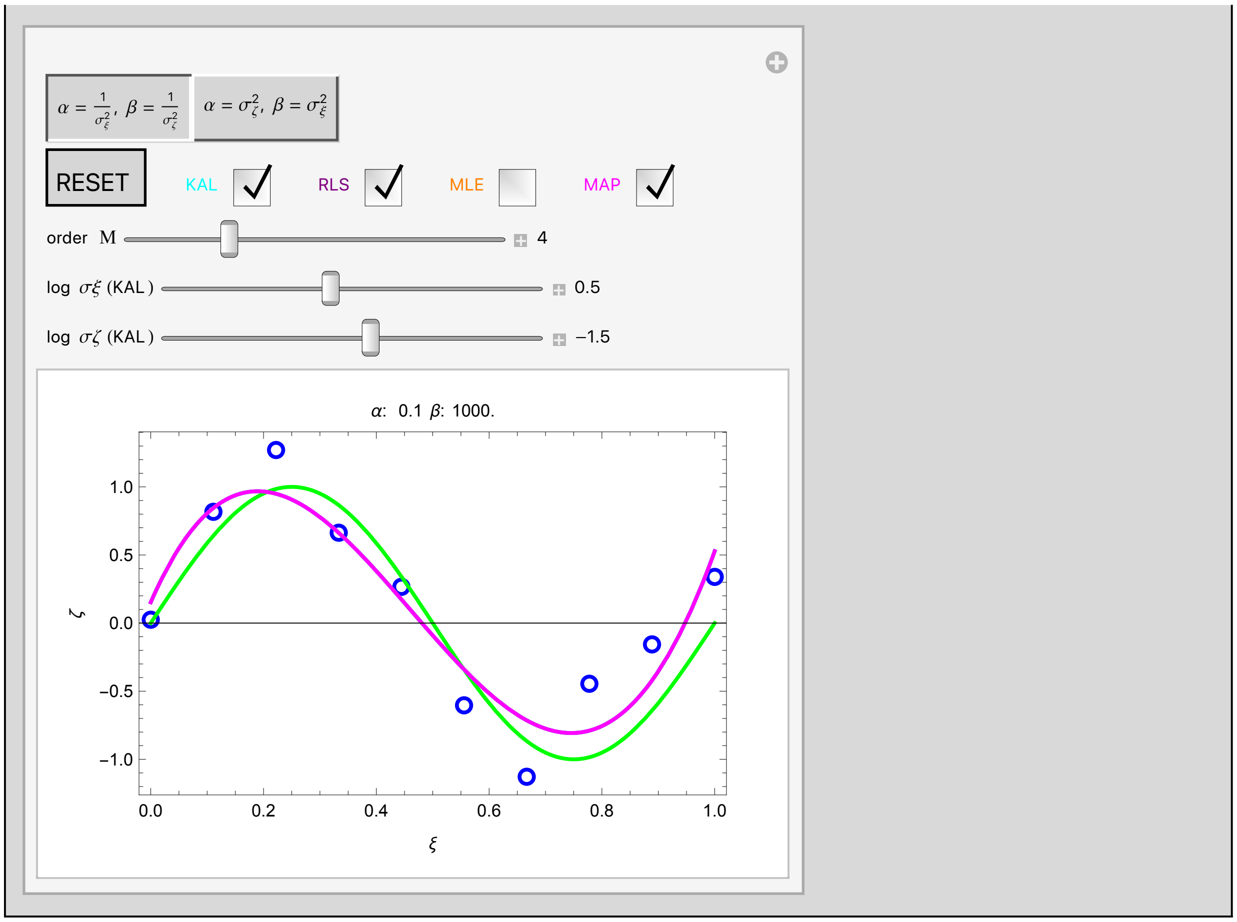
Wrap RLS in `Quiet` to suppress warnings. There is no free lunch; MAP also shows ill-conditioning and is similarly wrapped.

Recurrent RLS Fitting Procedure

In[73]:=
```
ClearAll[rrlsFit];
rrlsFit[σ2ζ_, 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[√σ2ζ IdentityMatrix[1]],
       {ξ0, Λ0},
       {List /@ ys, List /@ partialsFn[M, xs]}ᵀ];
     {ξ / √σ2ζ , Λ}]]];
```

In[75]:=
```
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, σξ2], β = If[αβBishop, 1/σζ2, σζ2]},
      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}]}}, (* green for ground truth *)
         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_ξ^2, β = 1/σ_ζ^2", False → "α = σ_ζ^2, β = σ_ξ^2"}],
    Row[{Button["RESET", (M = 4; logσξ = .5; logσζ = -1.5) &],
      Control[{{kalQ, True, Style["         KAL", Bold, Cyan]}, {True, False}}],
      Control[
       {{rlsQ, True, Style["         RLS", Bold, Purple]}, {True, False}}],
      Control[
       {{mleQ, False, Style["         MLE", Bold, Orange]}, {True, False}}],
      Control[{{mapQ, True, Style["         MAP", Bold, Magenta]},
        {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[75]=

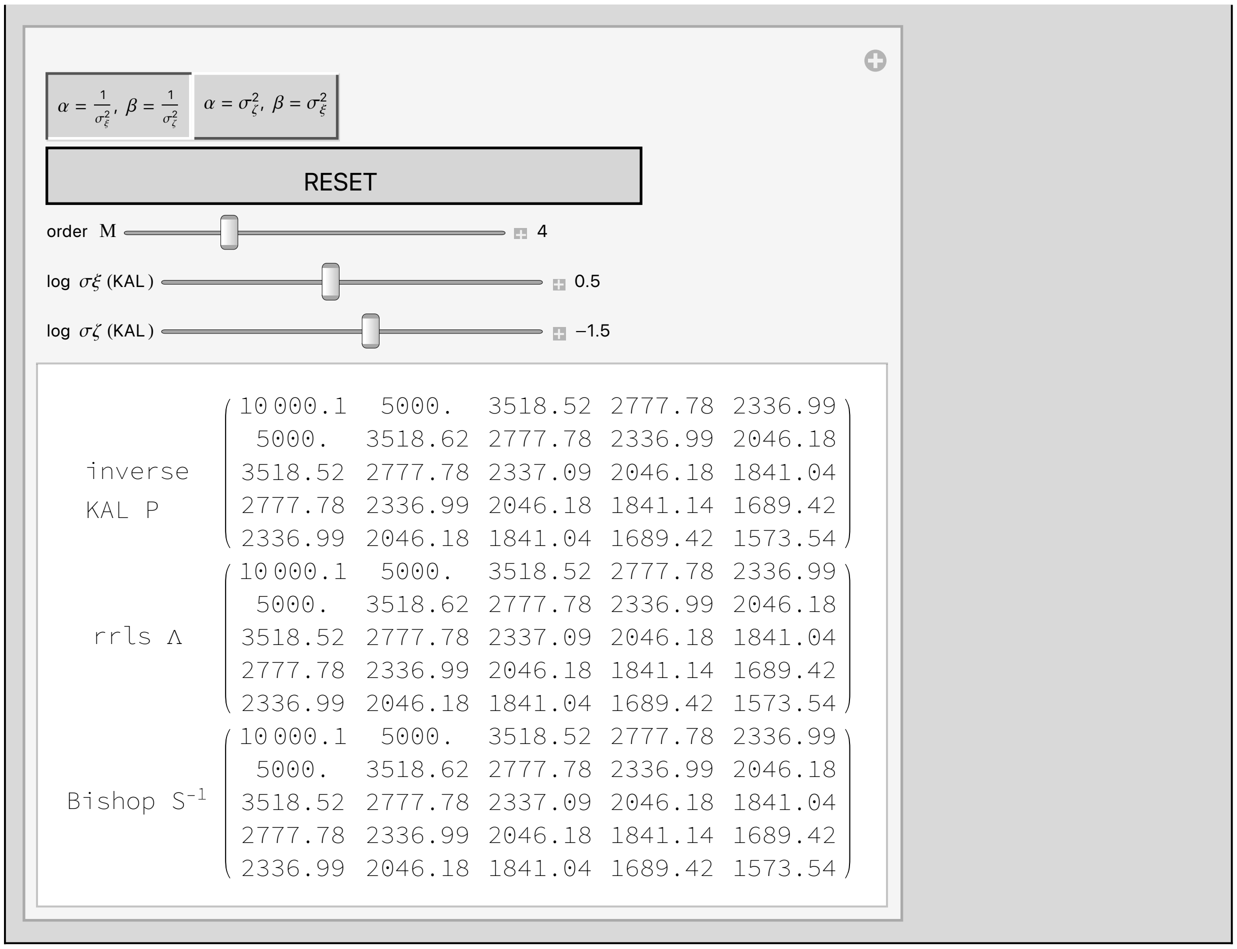

$\alpha = \frac{1}{\sigma_\xi^2}, \beta = \frac{1}{\sigma_\zeta^2}$
$\alpha = \sigma_\zeta^2, \beta = \sigma_\xi^2$
RESET
KAL ✓
RLS ✓
MLE
MAP ✓
order M 4
log σξ (KAL) 0.5
log σζ (KAL) −1.5
α: 0.1 β: 1000.
ζ
ξ

Covariance and Information Matrices

Notice that Bishop' s S^{-1} is different when α and β are swapped and inverted; it’s only an information matrix when α and β have their original assignments as $1/\sigma_\xi^2$ and $1/\sigma_\zeta^2$, respectively. The meaning of S^{-1} under the swapped and inverted assignments of α and β has not been explored.

In[76]:=
```
DynamicModule[{αβBishop = True},
 Manipulate[Module[{x},
   With[{cs = ϕ[M] /@ List /@ bts⟦1⟧, ts = bts⟦2⟧, σζ2 = 10.^(2 logσζ), σξ2 = 10.^(2 logσξ)},
    With[{kalman = kalFit[σζ2, σξ2][M, bts],
      rrls = Quiet@rrlsFit[σζ2, σξ2][M, bts]},
     With[{α = If[αβBishop, 1/σζ2, σζ2], β = If[αβBishop, 1/σξ2, σξ2]},
      Grid[( "inverse\nKAL P"  MatrixForm[Inverse[kalman⟦2⟧]]
                "rrls Λ"            MatrixForm[rrls⟦2⟧]
              "Bishop S^-1"     MatrixForm[sInv[α, β, cs, M]] )] ]]]],
  Column[{SetterBar[Dynamic[αβBishop],
     {True → "α = 1/σ_ζ^2, β = 1/σ_ξ^2", False → "α = σ_ζ^2, β = σ_ξ^2"}],
    Row[{Button["RESET", (M = 4;
         logσξ = .5;
         logσζ = -1.5) &]}, 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[76]=


$\alpha = \frac{1}{\sigma_\xi^2}, \beta = \frac{1}{\sigma_\zeta^2}$
$\alpha = \sigma_\zeta^2, \beta = \sigma_\xi^2$
RESET

order M 4

log σξ (KAL) 0.5

log σζ (KAL) −1.5

inverse KAL P
$$\begin{pmatrix} 10000.1 & 5000. & 3518.52 & 2777.78 & 2336.99 \\ 5000. & 3518.62 & 2777.78 & 2336.99 & 2046.18 \\ 3518.52 & 2777.78 & 2337.09 & 2046.18 & 1841.04 \\ 2777.78 & 2336.99 & 2046.18 & 1841.14 & 1689.42 \\ 2336.99 & 2046.18 & 1841.04 & 1689.42 & 1573.54 \end{pmatrix}$$

rrls Λ
$$\begin{pmatrix} 10000.1 & 5000. & 3518.52 & 2777.78 & 2336.99 \\ 5000. & 3518.62 & 2777.78 & 2336.99 & 2046.18 \\ 3518.52 & 2777.78 & 2337.09 & 2046.18 & 1841.04 \\ 2777.78 & 2336.99 & 2046.18 & 1841.14 & 1689.42 \\ 2336.99 & 2046.18 & 1841.04 & 1689.42 & 1573.54 \end{pmatrix}$$

Bishop S^{-1}
$$\begin{pmatrix} 10000.1 & 5000. & 3518.52 & 2777.78 & 2336.99 \\ 5000. & 3518.62 & 2777.78 & 2336.99 & 2046.18 \\ 3518.52 & 2777.78 & 2337.09 & 2046.18 & 1841.04 \\ 2777.78 & 2336.99 & 2046.18 & 1841.14 & 1689.42 \\ 2336.99 & 2046.18 & 1841.04 & 1689.42 & 1573.54 \end{pmatrix}$$

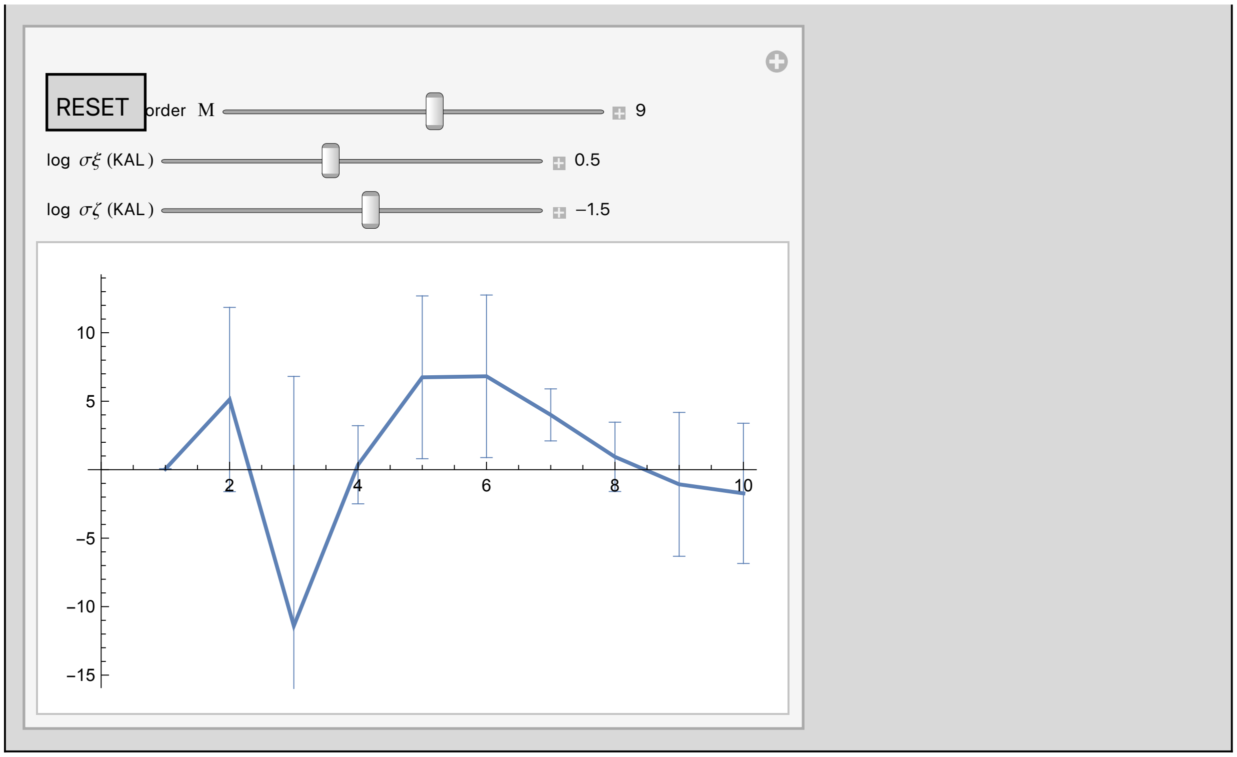
Covariance of the Prediction

The following shows estimated coefficients with their error bars. To translate from covariance of the estimate to covariance of the prediction, observe that the prediction is a linear combination of the estimates. Following https://stats.stackexchange.com/questions/160230, the covariance of the prediction at each input x is $a(x)\,P\,(a\,(x))^{\mathsf{T}}$. Bishop adds the fixed observation covariance σ_ζ^2 to the covariance of the prediction.

In[77]:=

```
Manipulate[Module[{x},
  With[{terms = symbolicPowers[x, M],
    σζ2 = 10.^(2 logσζ), σξ2 = 10.^(2 logσξ)},
   With[{k = kalFit[σζ2, σξ2][M, bts]},
    With[{δξ = Sqrt@Diagonal[k[[2]]],
      ξ = Flatten@k[[1]]},
     With[{eds = {ξ, δξ}ᵀ},
      Show[{ListPlot[Around /@ eds, Joined → True]}]]]]]],
 Column[{
   Row[{Button["RESET", (M = 9; logσξ = .5; logσζ = -1.5) &],
     Control[{{M, 9, "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[77]=



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

In[78]:=

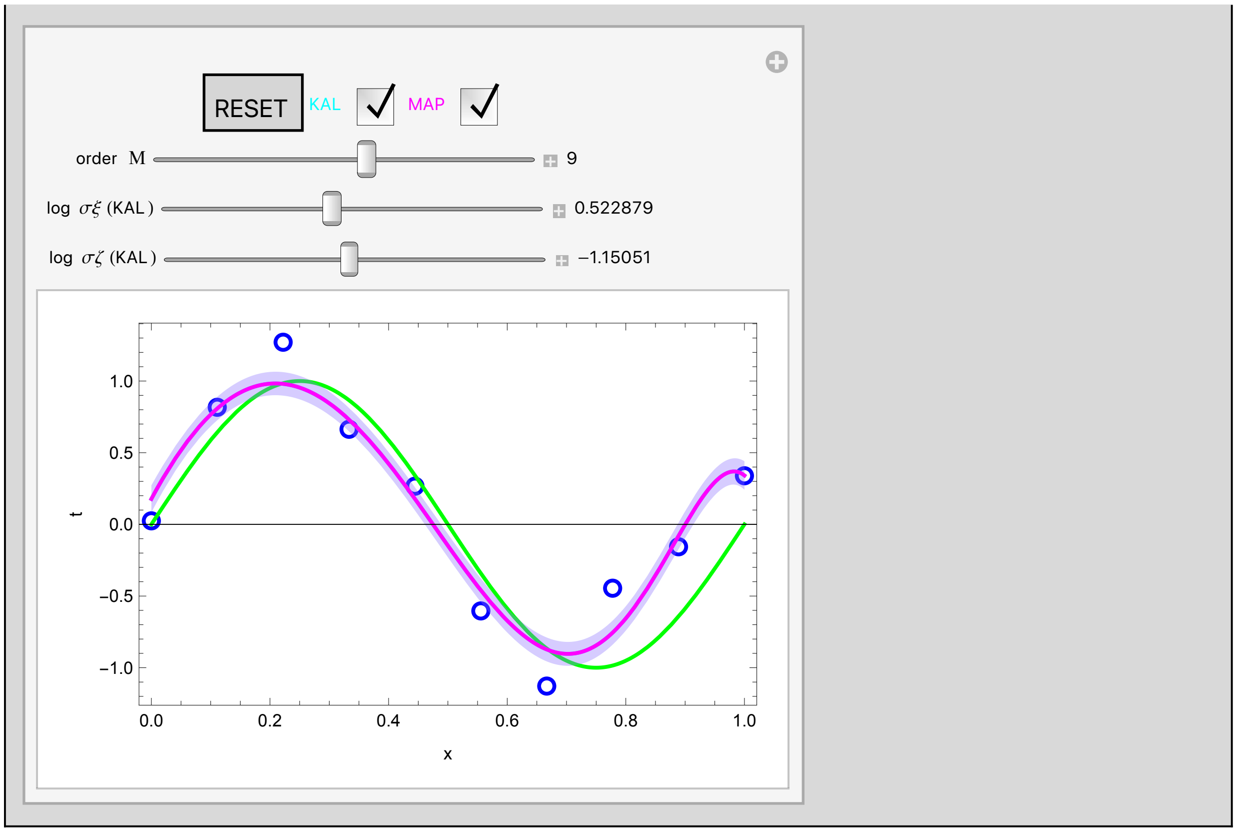
```
ClearAll[mapsSquared];
mapsSquared[α_, β_, x_, cs_, M_] :=
  With[{a = ϕ[M][x]},
   β⁻¹ + {a}.LinearSolve[sInv[α, β, cs, M], List /@ a]];
```

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. Bishop’s Equation 1.71 equals $\sigma_\zeta^2 + a_{\text{row}}(x) \cdot P \cdot a_{\text{row}}(x)^{\mathsf{T}}$.

In[80]:=

```
Manipulate[Module[{x, Σ2Fn},
  With[{terms = symbolicPowers[x, M],
     cs = ϕ[M] /@ List /@ bts⟦1⟧, ts = bts⟦2⟧, σ2ξ = 10^(2 logσξ), σ2ζ = 10^(2 logσζ)},
    With[{kalman = kalFit[σ2ζ, σ2ξ][M, bts]},
     With[{kalFn = {terms}.kalman⟦1⟧,
        bs2 = mapsSquared[1/σ2ξ, 1/σ2ζ, x, cs, M],
        mapFn = Quiet@mapMean[σ2ζ, σ2ξ, x, cs, ts, M]},
      Σ2Fn = σ2ζ + ({terms}.kalman⟦2⟧.{terms}ᵀ)⟦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[kalQ, AppendTo[showlist,
           Plot[{kalFn, kalFn + √Σ2Fn , kalFn - √Σ2Fn }, {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 ];
          logσζ = Log10[√0.005 ]) &],
       Control[{{kalQ, True, Style["KAL", Bold, Cyan]}, {True, False}}],
       Control[{{mapQ, True, Style["MAP", Bold, Magenta]}, {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[{{logσζ, Log10[√0.005 ], "log σζ (KAL)"},
      -5, 3, Appearance → "Labeled"}]}}]]
```

Out[80]=



Policy Gradient is co-RLS, co-KAL

In linear algebra, vectors are columns, i.e., $n \times 1$ matrices, and co-vectors 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).

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

$$\begin{aligned} &\gamma \leftarrow ([\gamma \cdot \Lambda] + [\omega \cdot \theta^{\intercal}]).(\Lambda + [\theta \cdot \theta^{\intercal}])^{-1} \\ &\Lambda \leftarrow (\Lambda + [\theta \cdot \theta^{\intercal}]) \end{aligned} \tag{14}$$

straight transposes of Equation 3. `LinearSolve` operates on the transposed right-hand side of the recurrence. Transpose the solution to get the recurrence. Apply the resulting dual model to the transpose of the original data. The following function is the dual of RLS update, and the fold effects co-

RLS. We check it against our running slope-intercept example. We have shown that RLS is equivalent to KAL, thus co-RLS is equivalent to co-KAL.

In[81]:=
```
ClearAll[coUpdate];
coUpdate[{γ_, Λ_}, {ω_, θ_}] :=
  With[{Π = (Λ + θ.θᵀ)},
   {LinearSolve[Π, Λ.γᵀ + θ.ωᵀ]ᵀ, Π}];
```

In[83]:=
```
MatrixForm /@ Fold[coUpdate,
  {( 0 0 ), (1.0*^-6     0   )},
            (  0     1.0*^-6 )
  {List /@ List /@ data, Transpose /@ List /@ partials}ᵀ]
```

Out[83]=
```
{( 0.503776  -0.277532 ), ( 280.356  119. )}
                          (  119.    119. )
```

This also awaits renormalization with prior information Λ_0. However, the renormalized equations will be obvious.

Finite-Difference Policy Gradient

The finite-difference method of policy-gradient is an instance of co-RLS (see http://www.scholarpedi-a.org/article/Policy_gradient_methods).

Imagine a *performance functional*, a scalar-valued function $J(\theta)$ of a column K-vector of policy parameters $\theta_{K\times 1}$. J measures how well a system performs on its tasks given the policy θ. The policy is often a deep learning network with K in the millions or billions. The objective of policy-gradient is to estimate the gradient co-vector $\nabla_\theta J_{1\times K}$, of J to feed it back into gradient-descent algorithms for improving the parameters.

Assemble a *batch* of $\mathcal{I}$ small, random policy-vector increments into a $K\times\mathcal{I}$ matrix, $\Delta\Theta_{K\times\mathcal{I}}$. This matrix represents a linear transformation of the co-vector $\nabla_\theta J_{1\times K}$ into a co-vector of a batch of $\mathcal{I}$ observed effects on the system, $\Delta J_{1\times\mathcal{I}}$, via the linear system $\nabla_\theta J_{1\times K}\cdot\Delta\Theta_{K\times\mathcal{I}} = \Delta J_{1\times\mathcal{I}}$. The gradient $\nabla_\theta J_{1\times K}$ takes the role of the Kalman state parameters we want to estimate. $\Delta\Theta$ takes the role of the Kalman partials of the model w.r.t. the sate parameters. The effects $\Delta J_{1\times\mathcal{I}}$ take the role of observations.

The Moore-Penrose ***right*** pseudoinverse RPI

$$\text{RPI} \overset{\text{def}}{=} (\Delta\Theta^{\mathsf{T}})_{\mathcal{I}\times K}\cdot(\Delta\Theta_{K\times\mathcal{I}}\cdot(\Delta\Theta^{\mathsf{T}})_{\mathcal{I}\times K})^{-1} \tag{15}$$

furnishes a large-memory, slow, numerically hazardous solution of the problem:

$$\nabla_\theta J_{\mathcal{I}\times 1}\cdot\Delta\Theta_{K\times\mathcal{I}}.\text{RPI} = \Delta J_{\mathcal{I}\times 1}.\text{RPI} \approx \text{est}\,(\nabla_\theta J_{\mathcal{I}\times 1}). \tag{16}$$

This is really nasty to implement if K is in the millions or billions, but co-KAL or co-RLS (Equation 7) easily beat it. Just as Kalman folding replaces the normal equations, so any straight transpose of KAL or RLS folding can replace RPI.

Padé Approximant via NIST

A Padé approximant is a ratio of two polynomials, where the bias term in the denominator is unity to prevent division by zero. Quoting from Srini Kumar and Bob Horton https://blog.revolutionanalytics.-com/2017/04/fitting-rational-functions-with-lm.html:

$$R(x) = \frac{\sum_{j=0}^{m} a_j\, x^j}{1 + \sum_{k=1}^{n} b_k\, x^k} = \frac{a_0 + a_1\, x + a_2\, x^2 + \cdots + a_m\, x^m}{1 + b_1\, x + b_2\, x^2 + \cdots + b_n\, x^n} \tag{17}$$

The following example from NIST (https://www.itl.nist.gov/div898/strd/nls/data/LINKS/DATA/Thurber.dat, edited to remove some blank lines) lets us illustrate:

```
NIST/ITL StRD
Dataset Name:  Thurber           (Thurber.dat)

File Format:   ASCII
               Starting Values   (lines 41 to 47)
               Certified Values  (lines 41 to 52)
               Data              (lines 61 to 97)

Procedure:     Nonlinear Least Squares Regression

Description:   These data are the result of a NIST study involving
               semiconductor electron mobility.  The response
               variable is a measure of electron mobility, and the
               predictor variable is the natural log of the density.

Reference:     Thurber, R., NIST (197?).
               Semiconductor electron mobility modeling.

Data:          1 Response Variable  (y = electron mobility)
               1 Predictor Variable (x = log[density])
               37 Observations
               Higher Level of Difficulty
               Observed Data

Model:         Rational Class (cubic/cubic)
               7 Parameters (b1 to b7)

               y = (b1 + b2*x + b3*x**2 + b4*x**3) /
                   (1 + b5*x + b6*x**2 + b7*x**3)  +  e

          Starting Values                  Certified Values
```

```
           Start 1     Start 2           Parameter     Standard Deviation
  b1 =   1000        1300           1.2881396800E+03  4.6647963344E+00
  b2 =   1000        1500           1.4910792535E+03  3.9571156086E+01
  b3 =    400         500           5.8323836877E+02  2.8698696102E+01
  b4 =     40          75           7.5416644291E+01  5.5675370270E+00
  b5 =      0.7         1           9.6629502864E-01  3.1333340687E-02
  b6 =      0.3         0.4         3.9797285797E-01  1.4984928198E-02
  b7 =      0.03        0.05        4.9727297349E-02  6.5842344623E-03

Residual Sum of Squares:                      5.6427082397E+03
Residual Standard Deviation:                  1.3714600784E+01
Degrees of Freedom:                                  30
Number of Observations:                              37

Data:   y             x
      80.574E0      -3.067E0
      84.248E0      -2.981E0
      87.264E0      -2.921E0
      87.195E0      -2.912E0
      89.076E0      -2.840E0
      89.608E0      -2.797E0
      89.868E0      -2.702E0
      90.101E0      -2.699E0
      92.405E0      -2.633E0
      95.854E0      -2.481E0
     100.696E0      -2.363E0
     101.060E0      -2.322E0
     401.672E0      -1.501E0
     390.724E0      -1.460E0
     567.534E0      -1.274E0
     635.316E0      -1.212E0
     733.054E0      -1.100E0
     759.087E0      -1.046E0
     894.206E0      -0.915E0
     990.785E0      -0.714E0
    1090.109E0      -0.566E0
    1080.914E0      -0.545E0
    1122.643E0      -0.400E0
    1178.351E0      -0.309E0
    1260.531E0      -0.109E0
    1273.514E0      -0.103E0
    1288.339E0       0.010E0
    1327.543E0       0.119E0
    1353.863E0       0.377E0
    1414.509E0       0.790E0
    1425.208E0       0.963E0
    1421.384E0       1.006E0
    1442.962E0       1.115E0
    1464.350E0       1.572E0
```

```
        1468.705E0        1.841E0
        1447.894E0        2.047E0
        1457.628E0        2.200E0
```

Read the Data into Mathematica

In[84]:=
```
nistData$ =
  "    80.574E0      -3.067E0
      84.248E0      -2.981E0
      87.264E0      -2.921E0
      87.195E0      -2.912E0
      89.076E0      -2.840E0
      89.608E0      -2.797E0
      89.868E0      -2.702E0
      90.101E0      -2.699E0
      92.405E0      -2.633E0
      95.854E0      -2.481E0
     100.696E0      -2.363E0
     101.060E0      -2.322E0
     401.672E0      -1.501E0
     390.724E0      -1.460E0
     567.534E0      -1.274E0
     635.316E0      -1.212E0
     733.054E0      -1.100E0
     759.087E0      -1.046E0
     894.206E0      -0.915E0
     990.785E0      -0.714E0
    1090.109E0      -0.566E0
    1080.914E0      -0.545E0
    1122.643E0      -0.400E0
    1178.351E0      -0.309E0
    1260.531E0      -0.109E0
    1273.514E0      -0.103E0
    1288.339E0       0.010E0
    1327.543E0       0.119E0
    1353.863E0       0.377E0
    1414.509E0       0.790E0
    1425.208E0       0.963E0
    1421.384E0       1.006E0
    1442.962E0       1.115E0
    1464.350E0       1.572E0
    1468.705E0       1.841E0
    1447.894E0       2.047E0
    1457.628E0       2.200E0";
```

In[85]:=
```
(nistTrainingSet$ = Transpose[
    nistDataPoints$ = Reverse /@ ReadList[
        StringToStream[nistData$],
        {Number, Number}]]) // MatrixForm
```
Out[85]//MatrixForm=
```
( -3.067  -2.981  -2.921  -2.912  -2.84   -2.797  -2.702  -2.699  -2.633  -2.481  -2.36
( 80.574  84.248  87.264  87.195  89.076  89.608  89.868  90.101  92.405  95.854  100.6
```

Symbolic Model

With the notation of the NIST example, rather than that of Kumar and Horton:

In[86]:=
```
ClearAll[x, y]
```

In[87]:=
```
nistModelPre$ =
 ReadList[StringToStream[StringReplace["y = (b1 + b2*x + b3*x**2 + b4*x**3) /
                   (1 + b5*x + b6*x**2 + b7*x**3)", "**" → "^"]]][[1]]
```
Out[87]=

$$\frac{b1 + b2\ x + b3\ x^2 + b4\ x^3}{1 + b5\ x + b6\ x^2 + b7\ x^3}$$

In[88]:=
```
nistDenominator$ = nistModelPre$[[2, 1]]
```
Out[88]=

$1 + b5\ x + b6\ x^2 + b7\ x^3$

In[89]:=
```
nistNumerator$ = nistModelPre$ * nistModelPre$[[2, 1]]
```
Out[89]=

$b1 + b2\ x + b3\ x^2 + b4\ x^3$

In[90]:=
```
ClearAll[e, y]
```

Linearized Model

Residual

In[91]:=
```
nistModel$ = nistNumerator$ - nistDenominator$ * y
```
Out[91]=

$b1 + b2\ x + b3\ x^2 + b4\ x^3 - \left(1 + b5\ x + b6\ x^2 + b7\ x^3\right)\ y$

Partials

```
In[92]:= A$[{x_, y_}] = (1 x x^2 x^3 -x y -x^2 y -x^3 y)
Out[92]=
{{1, x, x^2, x^3, -x y, -x^2 y, -x^3 y}}
```

```
In[93]:= ClearAll[ξ, ξ01, ξ02, Λ01, Λ02, P01, P02, certifiedξ, certifiedSqrtP]
```

Priors

```
In[94]:= (nistAPrioris$ = ReadList[StringToStream[
      "1000        1300           1.2881396800E+03   4.6647963344E+00
1000        1500          1.4910792535E+03   3.9571156086E+01
400         500          5.8323836877E+02   2.8698696102E+01
40          75          7.5416644291E+01   5.5675370270E+00
0.7         1          9.6629502864E-01   3.1333340687E-02
0.3         0.4        3.9797285797E-01   1.4984928198E-02
0.03        0.05       4.9727297349E-02   6.5842344623E-03"],
     {Number, Number, Number, Number}]^T) // MatrixForm
Out[94]//MatrixForm=
( 1000     1000     400      40       0.7        0.3        0.03       )
( 1300     1500     500      75       1          0.4        0.05       )
( 1288.14  1491.08  583.238  75.4166  0.966295   0.397973   0.0497273  )
( 4.6648   39.5712  28.6987  5.56754  0.0313333  0.0149849  0.00658423 )
```

Define global ξ01 as “Start1” priors in the NIST document:

```
In[95]:= (ξ01 = List /@ nistAPrioris$[[1]]) // MatrixForm
Out[95]//MatrixForm=
( 1000 )
( 1000 )
( 400  )
( 40   )
( 0.7  )
( 0.3  )
( 0.03 )
```

Define global ξ02 as “Start2” in the NIST document:

```
In[96]:= (ξ02 = List /@ nistAPrioris$⟦2⟧) // MatrixForm
Out[96]//MatrixForm=
 ⎛1300⎞
 ⎜1500⎟
 ⎜ 500⎟
 ⎜  75⎟
 ⎜   1⎟
 ⎜ 0.4⎟
 ⎝0.05⎠
```

"Certified Values" in the NIST document :

```
In[97]:= (certifiedξ = List /@ nistAPrioris$⟦3⟧) // MatrixForm
         (certifiedSqrtP = DiagonalMatrix@nistAPrioris$⟦4⟧) // MatrixForm
Out[97]//MatrixForm=
 ⎛ 1288.14  ⎞
 ⎜ 1491.08  ⎟
 ⎜ 583.238  ⎟
 ⎜ 75.4166  ⎟
 ⎜0.966295  ⎟
 ⎜0.397973  ⎟
 ⎝0.0497273 ⎠
Out[98]//MatrixForm=
 ⎛4.6648    0.       0.       0.        0.         0.          0.      ⎞
 ⎜  0.    39.5712    0.       0.        0.         0.          0.      ⎟
 ⎜  0.      0.    28.6987     0.        0.         0.          0.      ⎟
 ⎜  0.      0.       0.    5.56754      0.         0.          0.      ⎟
 ⎜  0.      0.       0.       0.    0.0313333      0.          0.      ⎟
 ⎜  0.      0.       0.       0.        0.     0.0149849       0.      ⎟
 ⎝  0.      0.       0.       0.        0.         0.      0.00658423 ⎠
```

Input collection for recurrent form:

```
In[99]:= (nistDataAndPartialsStream$ = {#⟦2⟧, A$[#]} & /@ nistDataPoints$) // MatrixForm
Out[99]//MatrixForm=
 80.574    {{1, -3.067, 9.40649, -28.8497, 247.12, -757.918, 2324.54}}
 84.248    {{1, -2.981, 8.88636, -26.4902, 251.143, -748.658, 2231.75}}
 87.264    {{1, -2.921, 8.53224, -24.9227, 254.898, -744.557, 2174.85}}
 87.195    {{1, -2.912, 8.47974, -24.693, 253.912, -739.391, 2153.11}}
 89.076    {{1, -2.84, 8.0656, -22.9063, 252.976, -718.451, 2040.4}}
 89.608    {{1, -2.797, 7.82321, -21.8815, 250.634, -701.022, 1960.76}}
 89.868    {{1, -2.702, 7.3008, -19.7268, 242.823, -656.109, 1772.81}}
 90.101    {{1, -2.699, 7.2846, -19.6611, 243.183, -656.35, 1771.49}}
 92.405    {{1, -2.633, 6.93269, -18.2538, 243.302, -640.615, 1686.74}}
 95.854    {{1, -2.481, 6.15536, -15.2715, 237.814, -590.016, 1463.83}}
100.696    {{1, -2.363, 5.58377, -13.1944, 237.945, -562.263, 1328.63}}
 101.06    {{1, -2.322, 5.39168, -12.5195, 234.661, -544.884, 1265.22}}
401.672    {{1, -1.501, 2.253, -3.38175, 602.91, -904.967, 1358.36}}
390.724    {{1, -1.46, 2.1316, -3.11214, 570.457, -832.867, 1215.99}}
567.534    {{1, -1.274, 1.62308, -2.0678, 723.038, -921.151, 1173.55}}
635.316    {{1, -1.212, 1.46894, -1.78036, 770.003, -933.244, 1131.09}}
733.054    {{1, -1.1, 1.21, -1.331, 806.359, -886.995, 975.695}}
759.087    {{1, -1.046, 1.09412, -1.14445, 794.005, -830.529, 868.734}}
894.206    {{1, -0.915, 0.837225, -0.766061, 818.198, -748.652, 685.016}}
990.785    {{1, -0.714, 0.509796, -0.363994, 707.42, -505.098, 360.64}}
1090.11    {{1, -0.566, 0.320356, -0.181321, 617.002, -349.223, 197.66}}
1080.91    {{1, -0.545, 0.297025, -0.161879, 589.098, -321.058, 174.977}}
1122.64    {{1, -0.4, 0.16, -0.064, 449.057, -179.623, 71.8492}}
1178.35    {{1, -0.309, 0.095481, -0.0295036, 364.11, -112.51, 34.7656}}
1260.53    {{1, -0.109, 0.011881, -0.00129503, 137.398, -14.9764, 1.63242}}
1273.51    {{1, -0.103, 0.010609, -0.00109273, 131.172, -13.5107, 1.3916}}
1288.34    {{1, 0.01, 0.0001, 1. × 10^-6, -12.8834, -0.128834, -0.00128834}}
1327.54    {{1, 0.119, 0.014161, 0.00168516, -157.978, -18.7993, -2.23712}}
1353.86    {{1, 0.377, 0.142129, 0.0535826, -510.406, -192.423, -72.5435}}
1414.51    {{1, 0.79, 0.6241, 0.493039, -1117.46, -882.795, -697.408}}
1425.21    {{1, 0.963, 0.927369, 0.893056, -1372.48, -1321.69, -1272.79}}
1421.38    {{1, 1.006, 1.01204, 1.01811, -1429.91, -1438.49, -1447.12}}
1442.96    {{1, 1.115, 1.24323, 1.3862, -1608.9, -1793.93, -2000.23}}
1464.35    {{1, 1.572, 2.47118, 3.8847, -2301.96, -3618.68, -5688.56}}
1468.71    {{1, 1.841, 3.38928, 6.23967, -2703.89, -4977.85, -9164.23}}
1447.89    {{1, 2.047, 4.19021, 8.57736, -2963.84, -6066.98, -12419.1}}
1457.63    {{1, 2.2, 4.84, 10.648, -3206.78, -7054.92, -15520.8}}
```

Setup for RLS

Define a symbolic column vector of coefficients to estimate. Set up some arbitrary prior covariances. Set up rules for evaluating symbolic coefficients at given numerical values for plotting.

In[100]:=

```
ξ = (b1
     b2
     b3
     b4
     b5
     b6
     b7);

P01 = IdentityMatrix[7];
Λ01 = Inverse[P01];
P02 = IdentityMatrix[7];
Λ02 = Inverse[P02];
```

In[104]:=

```
ClearAll[ξrules];
ξrules[numericalξ_] := Map[Apply[Rule, #] &, MapThread[Join, {ξ, numericalξ}]];
```

TODO: Fix RLS so it can handle this scenario.

As usual, the observation noise, *sqrtP*Z, is a constant over the run.

In[106]:=

```
ClearAll[rlsUpdate];
rlsUpdate[sqrtPZ_][{ξ_, Λ_}, {ζ_, a_}] :=
  With[{sPZia = LinearSolve[sqrtPZ, a]},
   With[{Π = (Λ + sPZiaᵀ.sPZia)},
    (*Print["a"];Print[MatrixForm[a]];
    Print["ζ"];Print[MatrixForm[ζ]];
    Print["sPZia"];Print[MatrixForm[sPZia]];
    Print["sPZiaᵀ.sPZia"];Print[MatrixForm[sPZiaᵀ.sPZia]];
    Print["Λ.ξ"];Print[MatrixForm[Λ.ξ]];
    Print["sPZiaᵀ.ζ"];Print[MatrixForm[sPZiaᵀ.ζ]];
    Print["sPZiaᵀ.ζ+Λ.ξ"];Print[MatrixForm[sPZiaᵀ.ζ+Λ.ξ]];*)
    {LinearSolve[Π, (sPZiaᵀ.ζ + Λ.ξ)], Π}]];
```

Unit test of *rlsUpdate*:

In[108]:=

```
rlsUpdate[{{1.0}}][{ξ01, Inverse[P01]}, nistDataAndPartialsStream$⟦1⟧]
```

Out[108]=

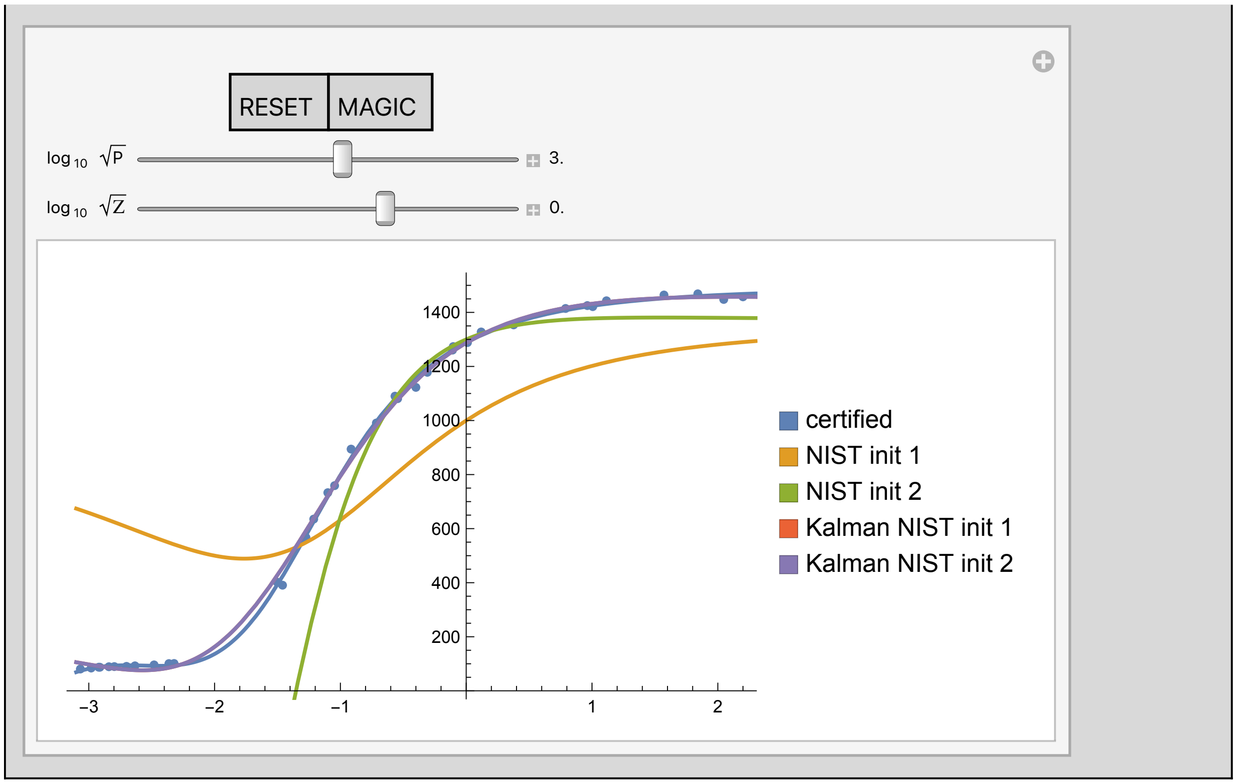
```
{{{0.999703 (1000.3 + 1. {{1.}, {-3.067}, {9.40649},
          {-28.8497}, {247.12}, {-757.918}, {2324.54}}.80.574)},
  {1.00091 (999.091 + 1. {{1.}, {-3.067}, {9.40649}, {-28.8497},
          {247.12}, {-757.918}, {2324.54}}.80.574)},
  {0.997209 (401.119 + 1. {{1.}, {-3.067}, {9.40649}, {-28.8497},
          {247.12}, {-757.918}, {2324.54}}.80.574)},
  {1.00856 (39.6631 + 1. {{1.}, {-3.067}, {9.40649}, {-28.8497},
          {247.12}, {-757.918}, {2324.54}}.80.574)},
  {0.926672 (0.730801 + 1. {{1.}, {-3.067}, {9.40649}, {-28.8497},
          {247.12}, {-757.918}, {2324.54}}.80.574)},
  {1.2249 (0.301976 + 1. {{1.}, {-3.067}, {9.40649}, {-28.8497},
          {247.12}, {-757.918}, {2324.54}}.80.574)},
  {0.310238 (-0.594222 + 1. {{1.}, {-3.067}, {9.40649}, {-28.8497},
          {247.12}, {-757.918}, {2324.54}}.80.574)}},
 {{2., -3.067, 9.40649, -28.8497, 247.12, -757.918, 2324.54},
  {-3.067, 10.4065,
   -28.8497, 88.482, -757.918,
   2324.54, -7129.35},
  {9.40649, -28.8497, 89.482, -271.374,
   2324.54, -7129.35, 21865.7},
  {-28.8497, 88.482, -271.374, 833.305,
   -7129.35, 21865.7, -67062.2},
  {247.12, -757.918, 2324.54, -7129.35,
   61069.5, -187297., 574440.},
  {-757.918, 2324.54, -7129.35, 21865.7, -187297.,
   574441., -1.76181 × 10^6},
  {2324.54, -7129.35, 21865.7, -67062.2, 574440.,
   -1.76181 × 10^6, 5.40347 × 10^6}}}
```

It turns out that the RLS update is slow and uninstructive. *kalmanUpdate* suffices to solve the problem.

In[109]:=

```
Manipulate[
 Module[{ξ1, P1, ξ2, P2, ξ3, Λ3, ξ4, Λ4},
  {ξ1, P1} = Fold[kalmanUpdate[{{10^(2 logσζ)}}], {ξ01, 10^(2 logσξ) P01},
    nistDataAndPartialsStream$];
  {ξ2, P2} = Fold[kalmanUpdate[{{10^(2 logσζ)}}], {ξ02, 10^(2 logσξ) P02},
    nistDataAndPartialsStream$];
  (* The following are slow and uninstructive: *)
  (*{ξ3,Λ3}=Fold[rlsUpdate[{{10^(2logσζ)}}],{ξ01,Inverse[10^(2logσξ)P01]},
    nistDataAndPartialsStream$];
  {ξ4,Λ4}=Fold[rlsUpdate[{{10^(2logσζ)}}],{ξ02,Inverse[10^(2logσξ)P02]},
    nistDataAndPartialsStream$];*)
  Show[{ListPlot[nistDataPoints$],
    Plot[{nistModelPre$ /. ξrules@certifiedξ, (*blue curve*)
      nistModelPre$ /. ξrules@ξ01, (* gold NIST init 1 *)
      nistModelPre$ /. ξrules@ξ02, (* green NITE init 2*)
      nistModelPre$ /. ξrules@ξ1, (* red Kalman NIST init 1*)
      nistModelPre$ /. ξrules@ξ2(*,(* purple Kalman NIST init 2 *)
      nistModelPre$/.ξrules@ξ3,
      nistModelPre$/.ξrules@ξ4*)
     },
     {x, -3.1, 2.3}, PlotLegends → SwatchLegend[{"certified", "NIST init 1",
        "NIST init 2", "Kalman NIST init 1", "Kalman NIST init 2"(*,
        "RLS NIST init 1","RLS NIST init 2"*)}]]}]],
 Grid[{
   {Row[{Button["RESET",
       (logσξ = 3.0; logσζ = 0.0) &],
      Button["MAGIC",
       (logσξ = 4.16; logσζ = 0.0) &]}]},
   {Control[{{logσξ, 3.0, "log₁₀ √P"}, -3, 8, Appearance → "Labeled"}]},
   {Control[{{logσζ, 0.0, "log₁₀ √Z"}, -6, 3, Appearance → "Labeled"}]}
  }]]
```

Out[109]=



We leave detailed examination of the covariances of this solution to future work.

Conclusion

Kalman folding (KAL) produces the same results as renormalized recurrent least squares (RLS) and as maximum a-posteriori (MAP) for appropriate choices of KAL and RLS covariances, or regularization hyperparameters for MAP.

Numerically and symbolically through order 3, MAP produces the same estimates as KAL and RLS, though not covariances, when its hyperparameters are swapped and inverted. MAP covariances are recovered in post-processing by un-swapping and re-inverting.

Finite-differences for policy gradient (FDPG) in reinforcement learning is co-RLS, co-KAL.

KAL and RLS have much better space-time efficiency than non-recurrent MAP. They avoid storing and multiplying large matrices. In all cases, we avoid matrix inverses by solving linear systems internally.