Homework

Stochastic Models and Adaptive Algorithms

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1 Linear regression

1.1 Function approximation with least squares

Ordinary least-squares

The best linear approximation of a function can be calculated using least-squares.

At first, a noisy sample of (x, y) pairs is generated such that $y_i = c\,x_i\,\sin(c\,x_i) + \epsilon_i$, where $\epsilon_i \sim \mathcal{N}(0, 1)$.

Let $[\mathbf{\Phi}]_{ij} = \mathrm{f}_j(x_i)$ be the transformed input vector and $\mathbf{y}$ the output, where f_j is a basis function. From this the $\mathbf{\Phi}(x)$ matrix can be generated after selecting a suitable f. A number of these were tried, and the best one for the problem seemed to be the polynomial one, that is $\mathrm{f}_i(x) = x^{i-1}$. As a parameter, $d = 10$ was used.

Now we have to find the optimal $\hat{\boldsymbol{\theta}}$ parameter vector, for which $\mathbf{\Phi}\,\boldsymbol{\theta} = \mathbf{y} = \begin{bmatrix} y_1 \dots y_n \end{bmatrix}^{\mathrm{T}}$. This is done like so: $\boldsymbol{\theta}^* \approx \hat{\boldsymbol{\theta}} = \mathbf{\Phi}^+\mathbf{y}$. The $\mathbf{\Phi}$ matrix of the sampled inputs and of the LS estimate are the same, so the function is evaluated at the same x values.

A computationally cheaper method for the pseudoinverse is QR decomposition. For this, the "economic" mode of scipy's `qr` function is used. Then the pseudoinverse is $\mathbf{\Phi}^+ = \mathbf{R}^{-1}\mathbf{Q}^{\mathrm{T}}$. Because the pseudoinverse of a matrix is unique, this method gives the same result as the previous one.

The results are shown in figure 1a.

Recursive least-squares

Next, more of the above described (x, y) pairs is sampled and $\hat{\boldsymbol{\theta}}_n$ calculated periodically using recursive least-squares. In the code, all of the samples are measured beforehand for simplicity.

The equation for $\hat{\boldsymbol{\theta}}$ can be reformulated in the following way:

$$\hat{\boldsymbol{\theta}} = \underbrace{\left[\sum_{i=1}^{n} \boldsymbol{\varphi}\,\boldsymbol{\varphi}^{\mathrm{T}}\right]^{-1}}_{\mathbf{\Psi}_n} \underbrace{\sum_{i=1}^{n} y_i\,\boldsymbol{\varphi}_i}_{z_n}. \tag{1}$$

Now we have an update rule for both $\mathbf{\Psi}_{n+1} = \left(\mathbf{\Psi} + \boldsymbol{\varphi}_{n+1}\boldsymbol{\varphi}_{n+1}{}^{\mathrm{T}}\right)^{-1}$, and $z_{n+1} = z_n + \boldsymbol{\varphi}_{n+1}\mathbf{y}_{n+1}$. Both $\mathbf{\Psi}_0$ and z_0 are set to zero. Also, in the code $\hat{\boldsymbol{\theta}}_n$ is calculated only when plotted for speed.

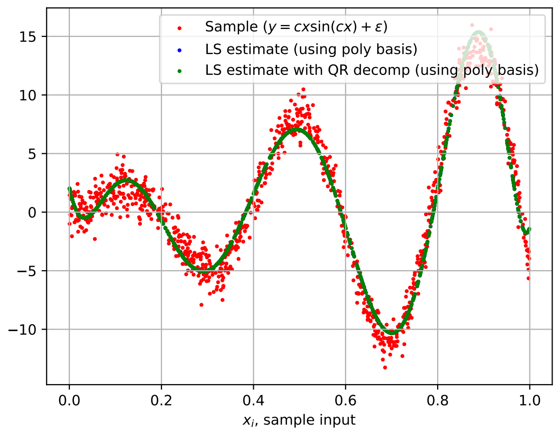
The resulting plots are shown in figure 1c., taken at $n \in [25, 50, 75, 100]$.

Least-norm problem

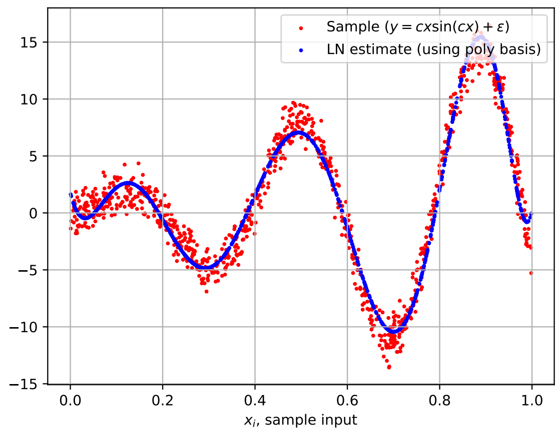
Now let's make $d > n$, specifically $n = 100$ and $d = 200$, which makes $\mathbf{\Phi}$ fat. We make the assumption that $\mathbf{\Phi}$ is still full-rank. The solution is the same, except we are going to use singular value decomposition (SVD) for the pseudoinverse of $\mathbf{\Phi}$.

The SVD is calculated like this: $\mathbf{\Phi}_{d\times n} = \mathbf{U}_{d\times d}\, \mathbf{\Sigma}_{d\times n}\, \mathbf{V}_{n\times n}{}^{\mathrm{T}}$. Let's denote the matrix of column vectors of the normalized eigen-vectors of matrix $\mathbf{\Phi}$ by $\mathrm{eig}(\mathbf{\Phi})$. Let's denote the eigenvalues by $\mathrm{eigval}(\mathbf{\Phi})$. Then, $\mathbf{U} = \mathrm{eig}(\mathbf{\Phi}\, \mathbf{\Phi}^{\mathrm{T}})$, $\mathbf{V} = \mathrm{eig}(\mathbf{\Phi}^{\mathrm{T}}\, \mathbf{\Phi})$ and $\mathbf{\Sigma} = \mathrm{diag}(\mathrm{eigval}(\mathbf{\Phi}\, \mathbf{\Phi}^{\mathrm{T}}))_{d\times n}$. Then, the pseudoinverse is $\mathbf{\Phi}^{+} = \mathbf{V}\, \mathbf{\Sigma}^{+}\, \mathbf{U}^{\mathrm{T}}$. For $\mathbf{\Sigma}^{+}$, we take the inverse of the non-zero elements of $\mathbf{\Sigma}$, and add zeros such that it has the shape of $d \times n$.

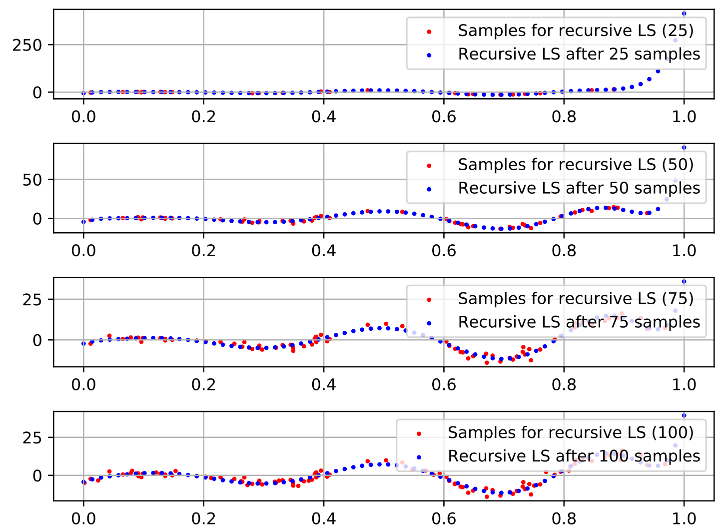
The resulting plots are shown in figure 1b.



(a) Least-squares estimate for thin $\mathbf{\Phi}$



(b) Least-norm estimate for fat $\mathbf{\Phi}$



(c) Recursive least-squares

Figure 1: Experiments with ordinary least-squares

1.2 Approximating auto-regressive series

A recursive time-series is generated from the give equation: $y_t = a\, y_{t-1} + b\, y_{t-2} + \epsilon_t$. Let's calculate the least-squares estimate using $\boldsymbol{\varphi}_t = \left[y_{t-1}, y_{t-2}\right]$, $\boldsymbol{\Phi} = \left[\boldsymbol{\varphi}_i \dots \boldsymbol{\varphi}_n\right]$. Then $\hat{\boldsymbol{\theta}} = \boldsymbol{\Phi}^+\, \mathbf{y}$.

The time plots can be seen on figure 2a.

Let's calculate the inverse of the covariance matrix:s $\boldsymbol{\Gamma}_n = \frac{1}{n}\, \boldsymbol{\Phi}^{\mathrm{T}}\, \boldsymbol{\Phi}$. Now define $\Delta\boldsymbol{\theta} := (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_n)$. The confidence ellipsoid is given by

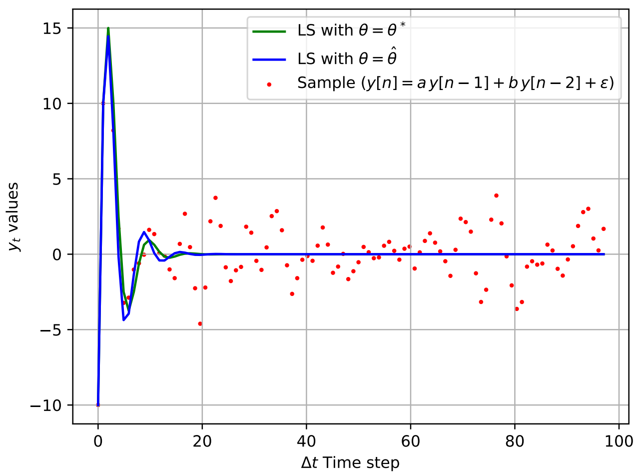
$$\Delta\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\Gamma}_n\Delta\boldsymbol{\theta} \leq \frac{q\, \hat{\sigma}_n^2}{n}, \tag{2}$$

where q is calculated from the inverse of the cumulative χ^2 distribution function given the p probabilities ($q = \mathrm{F}(p)^{-1}_{\chi^2(d)}$). In this problem, $d = 2$. Eq. 2 means that with probability p, the optimal $\boldsymbol{\theta}^*$ is at most $\Delta\boldsymbol{\theta}$ distance from $\hat{\boldsymbol{\theta}}$.

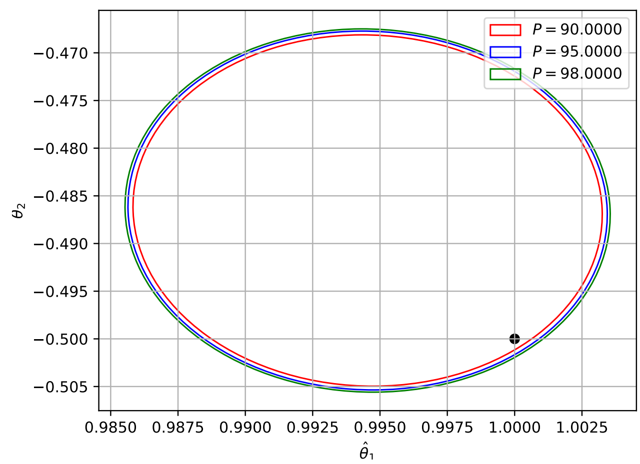
Now we assume that $\hat{\sigma}_n = 1$, and let $\Gamma_{ij}/n = [\boldsymbol{\Gamma}_n]_{ij}$. Then we have an equation that outputs an ellipse for a p probability. Written out:

$$\Delta\theta_1^2\, \Gamma_{11} + 2\, \Delta\theta_1\, \Delta\theta_2\, \Gamma_{12} + \Delta\theta_2^2\, \Gamma_{22} = q. \tag{3}$$

For the plotting, this equation is transformed so that the axis distances and the rotation angle is known with the function `ellipse_transform`[1].



(a) Time-series



(b) Confidence ellipsoids

Figure 2: Experiments with auto-regressive series

2 Kernel methods

3 Reinforcement learning

References

[1] Ellipse equation: https://www.maa.org/external_archive/joma/Volume8/Kalman/General.html#:~:text=Applying%20the%20methods%20of%20%EF%BF%BD,rotated%20through%20an%20angle%20%CE%B1%20.&text=which%20is%20in%20the%20form,with%20A%20and%20C%20positive.