

Problem 4.4

(a) Why do we normalize f ? In addition to answering the question about why we need to normalize f , also

prove that the term to normalize by is $\sqrt{\sum_{q=0}^{Q_f} \frac{1}{2q+1}}$

$$\rightarrow E_{a,x}[f^2] = E_{a,x}[(a_0L_0(x) + a_1L_1(x) + \dots + a_{Q_f}L_{Q_f}(x))^2]$$

$$\because \int_{-1}^1 L_k(x)L_l(x) dx = \begin{cases} 0, l \neq k \\ \frac{2}{2k+1}, l = k \end{cases} \text{ and } E_x[f(x)] = \int_a^b P(x)f(x)dx$$

$$\Rightarrow E_{a,x}[f^2] = E_a \left[\int_{-1}^1 \frac{1}{2} [(a_0L_0(x))^2 + (a_1L_1(x))^2 + \dots + (a_{Q_f}L_{Q_f}(x))^2] dx \right]$$

$$= E_a \left[\sum_{q=0}^{Q_f} \frac{a_q^2}{2q+1} \right]$$

$$= \frac{1}{1}E[a_0^2] + \frac{1}{3}E[a_1^2] + \frac{1}{5}E[a_2^2] + \dots + \frac{1}{2Q_f+1}E[a_{Q_f}^2]$$

$$\because \sigma^2 = 1, \text{ then } E[a_i^2] = \sigma^2 - (E[a_i])^2 = 1 - 0 = 1, \text{ for } i = 1, 2, \dots, Q_f$$

$$\Rightarrow \frac{1}{1}E[a_0^2] + \frac{1}{3}E[a_1^2] + \frac{1}{5}E[a_2^2] + \dots + \frac{1}{2Q_f+1}E[a_{Q_f}^2] = \frac{1}{1} + \frac{1}{3} + \frac{1}{5} + \dots + \frac{1}{2Q_f+1} = \sum_{q=0}^{Q_f} \frac{1}{2q+1}$$

$$\Rightarrow E_{a,x}[f^2] = \sum_{q=0}^{Q_f} \frac{1}{2q+1}$$

Letting this result to 1, the term can be normalized when each a_i , (for $i = 1, 2, \dots, Q_f$) is divided by the

normalizer $\sqrt{\sum_{q=0}^{Q_f} \frac{1}{2q+1}}$, that is, $\tilde{a}_i = \frac{a_i}{\sqrt{\sum_{q=0}^{Q_f} \frac{1}{2q+1}}}$.

The reason to normalize f is that normalizing $E_{a,x}[f^2] = 1$ let the noise level σ^2 automatically calibrated to the signal level.

(b) How can we obtain g_2 and g_{10} ?

Our target function is $f(x) = \sum_{q=0}^{Q_f} a_q L_q(x)$ and hypothesis is $g_d(x) = \sum_{i=0}^d w_i L_i(x)$. Therefore, 2-order

and 10-order polynomial model are $g_2(x) = \sum_{i=0}^2 w_i L_i(x) = w^T L$, $w, L \in R^3$ and $g_{10}(x) = \sum_{i=0}^{10} w_i L_i(x) = w^T L$, $w, L \in R^{11}$

In implementation,

```
z_train_2 = L(x_train, 2);
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z_train_10 = L(x_train, 10);
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```
w_2 = glmfit(z_train_2, y_train, 'normal', 'constant', 'off')
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```
w_10 = glmfit(z_train_10, y_train, 'normal', 'constant', 'off')
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```
g_2 = computeLegPoly(x_test, 2) * w_2
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```
g_10 = computeLegPoly(x_test, 10) * w_10
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(c) How can we compute E_{out} analytically for a given g_{10} ?

$$\begin{aligned}
E_{out} &= E_{x,\epsilon}[(g_{10}(x) - y)^2] \\
&= E_{x,\epsilon}[(g_{10}(x) - (f(x) + \sigma\epsilon))^2] \\
&= E_{x,\epsilon}[(g_{10}(x) - f(x)) - \sigma\epsilon]^2 \\
&= E_{x,\epsilon}[(g_{10}(x) - f(x))^2 - 2(g_{10}(x) - f(x))\sigma\epsilon + (\sigma\epsilon)^2] \\
&= E_{x,\epsilon}[(\sum_{i=0}^{10} w_i L_i(x) + \sum_{j=0}^{Q_f} a_j L_j(x))^2 - 2(\sum_{i=0}^{10} w_i L_i(x) - \sum_{j=0}^{Q_f} a_j L_j(x))\sigma\epsilon + (\sigma\epsilon)^2] \\
\because E_{\epsilon}[\epsilon] &= 0 \Rightarrow E_{x,\epsilon}[-2(\sum_{i=0}^{10} w_i L_i(x) - \sum_{j=0}^{Q_f} a_j L_j(x))\sigma\epsilon] = 0 \\
\because E_{\epsilon}[\epsilon^2] &= 1 \Rightarrow E_{x,\epsilon}[(\sigma\epsilon)^2] = \sigma^2 \\
\Rightarrow E_{out} &= E_{x,\epsilon}[(\sum_{i=0}^{10} w_i L_i(x) + \sum_{j=0}^{Q_f} a_j L_j(x))^2] \\
&= E_{x,\epsilon}[(\sum_{i=0}^{10} w_i L_i(x))^2 - 2\sum_{j=0}^{\min(10, Q_f)} (w_j a_j L_j(x))^2 + \sum_{k=0}^{Q_f} (a_k L_k(x))^2] \\
&= E_{\epsilon}[\sum_{i=0}^{10} \frac{w_i^2}{2i+1} - 2\sum_{j=0}^{\min(10, Q_f)} \frac{w_j a_j}{2j+1} + \sum_{k=0}^{Q_f} \frac{a_k^2}{2k+1}] \\
&= \sum_{i=0}^{10} \frac{w_i^2}{2i+1} - 2\sum_{j=0}^{\min(10, Q_f)} \frac{w_j a_j}{2j+1} + \sum_{k=0}^{Q_f} \frac{a_k^2}{2k+1}
\end{aligned}$$

(d) Vary Q_f, N, σ , where $Q_f \in \{5, 10, 15, 20\}$, $N \in \{40, 80, 120\}$, $\sigma^2 \in \{0, 0.5, 1.0, 1.5, 2.0\}$, run 500 of experiments for each combination of the parameters, each time computing $E_{out}(g_2)$ and $E_{out}(g_{10})$. Averaging these out-of-sample errors gives estimates of the expected out-of-sample error for the given learning scenario (Q_f, N, σ) using H_2 and H_{10} . Define the overfit measure $E_{out}(H_{10}) - E_{out}(H_2)$.

$$\begin{cases} E_{out}(H_2) &= \text{average over experiments } (E_{out}(g_2)) \\ E_{out}(H_{10}) &= \text{average over experiments } (E_{out}(g_{10})) \end{cases}$$

- When is the overfit measure significantly positive (i.e., the overfitting is serious) as opposed to significantly negative?

- Serious overfitting happens when using mean error measurement, model complexity Q_f is large, number of training data N is small and noise coefficient σ is large.

- How error measurement varies? Explain your observation.

- In general, error measurement grows (negatively) larger when model complexity Q_f and N goes larger.

- Given a sufficiently large N ($N=80$ or 120), the difference between complex model (H_{10}) and simple model (H_2) grows larger when model complexity Q_f grows larger.

- Without stochastic noise, error measurement is larger than those in the same N and Q_f but with stochastic noise.

- In general,

overfitting goes up when stochastic noise σ^2 goes up. (more obvious when N is small)

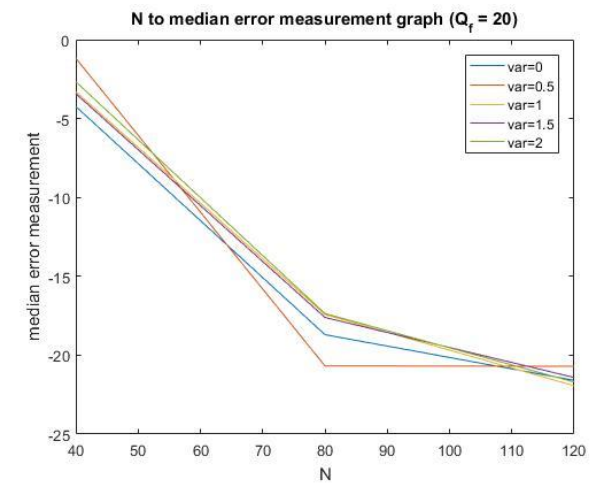
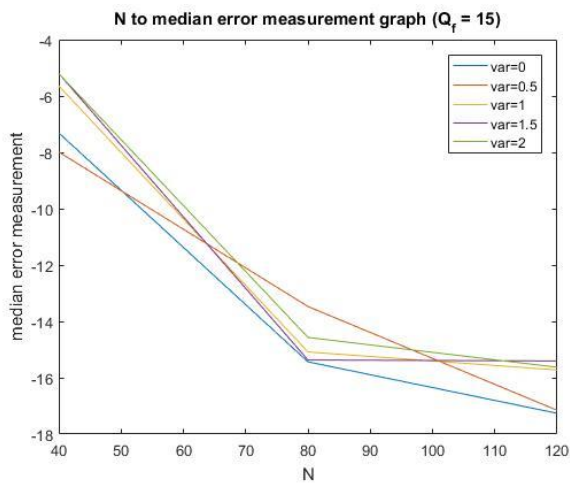
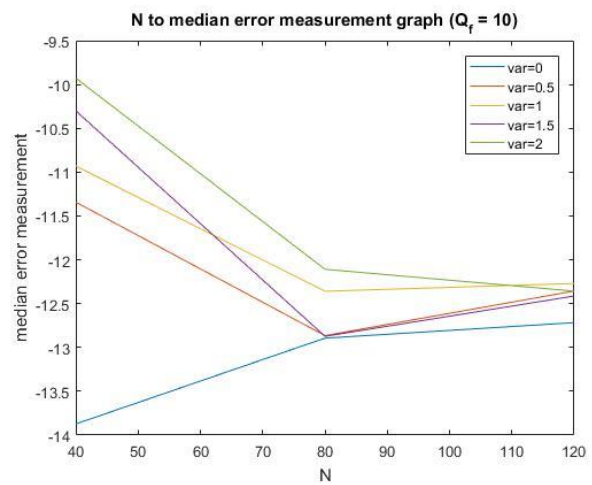
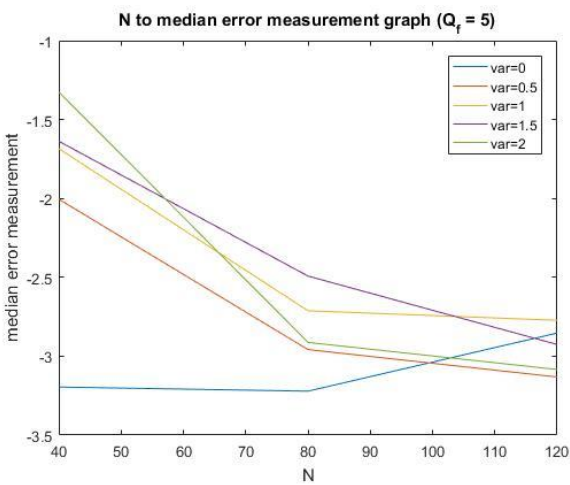
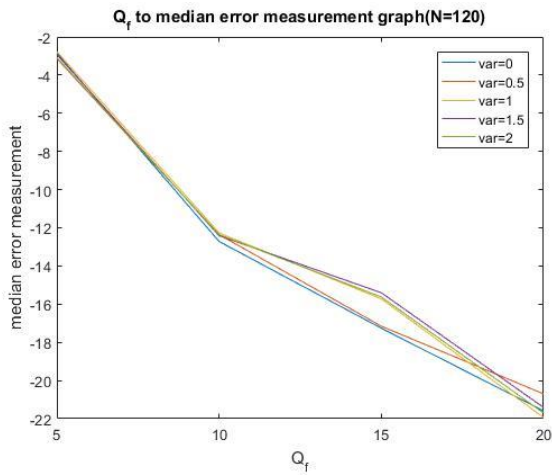
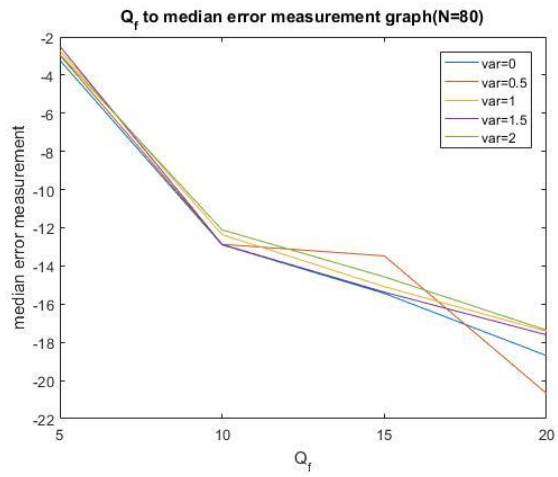
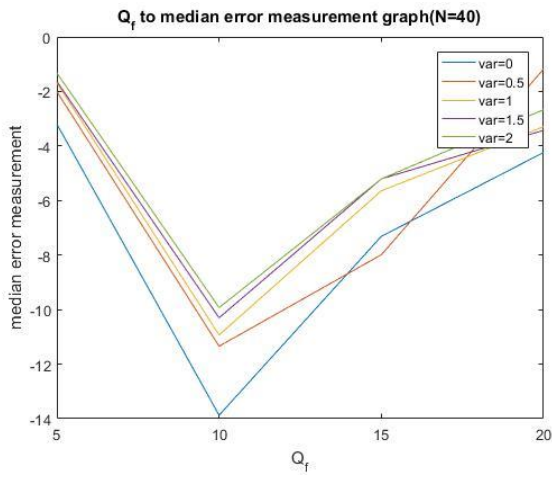
overfitting goes up when model complexity Q_f goes up.

overfitting goes down when number of training data N goes up.

Comments on your observation on the error measurement between mean and median.

- The result using mean error measurement goes very stable, because it counts very extreme case into average (e.g. very extreme positive or negative large ε or σ).

- Using median's result relatively consistent due to picking median value of the error measurement vector.



Result data (mean / median error measurement)

Mean error measurement				Median error measurement			
var = 0	N = 40	N = 80	N = 120	var = 0	N = 40	N = 80	N = 120
Qf = 5	-4.12172	-4.01457	-3.86343	Qf = 5	-3.19543	-3.22157	-2.85317
Qf = 10	-15.1925	-14.774	-13.9225	Qf = 10	-13.8729	-12.8938	-12.7172
Qf = 15	3338.675	-6.90773	-17.238	Qf = 15	-7.31356	-15.4362	-17.2614
Qf = 20	2845.974	0.950951	-23.483	Qf = 20	-4.23798	-18.6988	-21.5905
var = 0.5	N = 40	N = 80	N = 120	var = 0.5	N = 40	N = 80	N = 120
Qf = 5	48.0182	-3.74689	-4.00618	Qf = 5	-2.00527	-2.95798	-3.13175
Qf = 10	57.57465	-14.2847	-13.5448	Qf = 10	-11.343	-12.8651	-12.3565
Qf = 15	3565.225	-5.04213	-14.4552	Qf = 15	-7.98864	-13.4717	-17.1567
Qf = 20	1663.051	-0.5797	-18.165	Qf = 20	-1.18132	-20.68	-20.7001
var = 1.0	N = 40	N = 80	N = 120	var = 1.0	N = 40	N = 80	N = 120
Qf = 5	209.6775	-2.94872	-3.66224	Qf = 5	-1.68482	-2.71218	-2.77246
Qf = 10	15.25814	-12.569	-13.6326	Qf = 10	-10.9303	-12.3592	-12.2701
Qf = 15	340.7107	-0.81053	-10.6132	Qf = 15	-5.64385	-15.0851	-15.7239
Qf = 20	2108.379	-8.60978	-21.6239	Qf = 20	-3.29368	-17.4243	-21.9367
var = 1.5	N = 40	N = 80	N = 120	var = 1.5	N = 40	N = 80	N = 120
Qf = 5	79.00667	-2.78508	-3.65293	Qf = 5	-1.6375	-2.49205	-2.92583
Qf = 10	49.38114	-14.3603	-14.0952	Qf = 10	-10.3007	-12.8735	-12.4134
Qf = 15	870.3479	0.403971	-16.1919	Qf = 15	-5.20563	-15.3705	-15.4035
Qf = 20	7970.857	3.369453	-21.0473	Qf = 20	-3.42507	-17.6101	-21.4139
var = 2.0	N = 40	N = 80	N = 120	var = 2.0	N = 40	N = 80	N = 120
Qf = 5	1157.489	-3.75437	-3.69793	Qf = 5	-1.32536	-2.91244	-3.08431
Qf = 10	279.0018	-12.8372	-13.5044	Qf = 10	-9.92836	-12.1084	-12.3572
Qf = 15	98481.64	-4.21175	-16.3296	Qf = 15	-5.20891	-14.5705	-15.6274
Qf = 20	7227.035	8.334017	-20.2116	Qf = 20	-2.67036	-17.3606	-21.7036