ANLY-601

Advanced Pattern Recognition

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Spring 2018

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L11 – Map Estimates, Bayesian Inference, Hyperparameter Choice

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Continuing with Bayesian Methods

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MAP Estimates, Bayesian Inference, and Hyperparameter Choice

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Why use a MAP Estimate, they're Biased?

Consider the expected squared error of any estimator:

$$MSE = E\left[(\bar{\mu}-\mu)^2\right] = E\left[\left\{(\bar{\mu}-E[\bar{\mu}]) + (E[\bar{\mu}]-\mu)\right\}^2\right]$$

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$$= \quad E\left[(\bar{\mu}-E[\bar{\mu}])^2\right] + (E[\bar{\mu}]-\mu)^2$$

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$$= \quad \mathrm{var}(\bar{\mu}) + bias^2$$

Bias isn't the only consideration - variance is also important. There's usually a trade-off; increase the bias, and the variance drops, and vice-versa.

Bias-Variance Trade-Off and MAP Estimates

Let's go back to our MAP estimate of the mean for Gaussian data:

$$\bar{\mu} = \frac{m\lambda^2}{m\lambda^2 + \sigma^2} \frac{1}{m} \sum_{i=1}^{m} x_i + \frac{\sigma^2}{m\lambda^2 + \sigma^2} \mu_0$$

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The bias and variance are (show these!)

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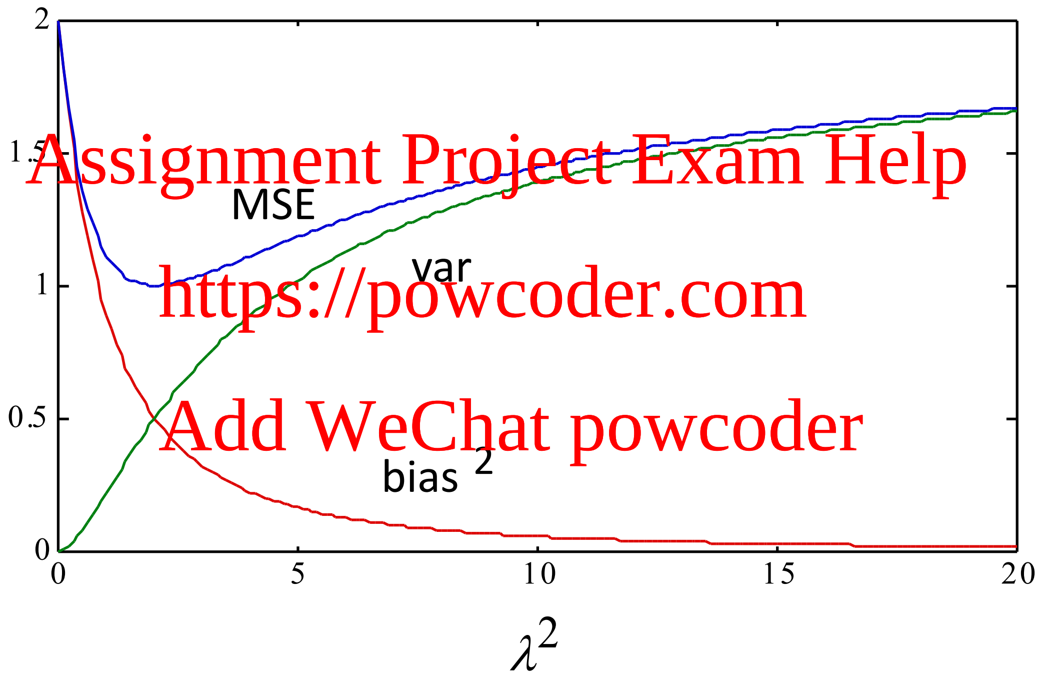
$$bias^2 = (E[\bar{\mu}] - \mu)^2 = \left(\frac{\sigma^2}{m\lambda^2 + \sigma^2} (\mu_0 - \mu) \right)^2$$

$$\mathrm{var}(\bar{\mu}) = E\left[(\bar{\mu} - E[\bar{\mu}])^2 \right] = \left(\frac{m\lambda^2}{m\lambda^2 + \sigma^2} \right)^2 \frac{\sigma^2}{m}$$

As $m \rightarrow \infty$ both go to zero

Bias-Variance Trade-Off and MAP Estimates

The curves look like this



The curve of MSE has its minimum at
a non-zero value of λ. Specifically -- $\lambda_{opt}{}^2 = (\mu_0 - \mu)^2$

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MAP Estimates and Regularizers

The log of the posterior on the parameters is

$$\log\left(p(\Theta \mid D)\right) = \log\left(p(D \mid \Theta)\right) + \log\left(p(\Theta)\right) - \log(p(D))$$

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log-likelihood – bare cost

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log prior -- regularizer

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We saw that maximizing the data log-likelihood is equivalent to minimizing some nice cost function -- e.g. the mean-squared-error.

Maximizing the log-posterior is equivalent to minimizing a regularized cost function. **The effect of the regularizer is to reduce the parameter variance at the cost of adding parameter bias**.

MAP Regression

One can use the MAP estimate of Θ, and construct the regression function

$$E[t \mid x, D] = f(t \mid x, \hat{\Theta})$$

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where $\hat{\Theta}$ is the value that maximizes the posterior p(Θ|D).

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One can also use this MAP value to estimate the target density

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$$p(t \mid x, \hat{\Theta}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp - \frac{1}{2\sigma^2}\left(t - f(t \mid x, \hat{\theta})\right)^2$$

Example of Map Regression – Ridge

Ridge regression uses a parameterized regressor $f(x,\Theta)$, the familiar SSE cost function (Gaussian likelihood for the targets), and a Gaussian prior on the parameters, typically centered at zero

$$p(\theta) = \frac{1}{\sqrt{2\pi / \Lambda^2}} \exp -\frac{1}{2/\Lambda^2} |\theta|^2$$

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The regularized cost function is thus

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$$E(\Lambda, \theta) = \sum_{i=1}^{N} \left(t_i - f(x_i, \theta)\right)^2 + \Lambda |\theta|^2$$

That for linear regression, $f(x,\Theta)$ is linear in Θ so E is quadratic in Θ and the cost function can be minimized in closed form (just like MLE estimation for linear regression).

Bayesian Estimation

Let's continue. Suppose we have obtained the posterior on the parameters p(Θ| D) and we wish to find the probability of a new data value x. A Bayesian says that you should calculate this from his version of the distribution p(x)

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$$p(x|D) = \int p(x\,|\,\Theta)\; p(\Theta\,|D)\, d\Theta$$

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A Bayesian computes the mean of any function f(x) as

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$$E\left[f\mid D\right] = \int f(x)\; p(x\,|\,D)\; dx = \iint f(x)\; p(x\,|\,\Theta)\; p(\Theta\,|\,D)\; d\Theta\; dx$$

Bayesian and MAP Estimates

Relation to **MAP** Estimates: Suppose the posterior is sharply peaked up about its maximum value (the MAP estimate). Write a series expansion of p(x|Θ) about the maximum and substitute into the integral

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$$p(x\,|\,D) = \int p(x\,|\,\Theta)\, p(\Theta\,|\,D)\, d\Theta = \int \left[p(x\,|\,\hat{\Theta}) + \left.\frac{dp(x\,|\,\Theta)}{d\Theta}\right|_{\hat{\Theta}} (\Theta - \hat{\Theta}) \right.$$

$$\left. + \frac{1}{2} \left.\frac{d^2 p(x\,|\,\Theta)}{d\Theta^2}\right|_{\hat{\Theta}} (\Theta - \hat{\Theta})^2 + \ldots \right] p(\Theta\,|\,D)\, d\Theta$$

$$= p(x\,|\,\hat{\Theta}) + \left.\frac{dp(x\,|\,\Theta)}{d\Theta}\right|_{\hat{\Theta}} E\left[(\Theta - \hat{\Theta})\,|\,D\right] + \frac{1}{2} \left.\frac{d^2 p(x\,|\,\Theta)}{d\Theta^2}\right|_{\hat{\Theta}} E\left[\left(\Theta - \hat{\Theta}\right)^2 |\,D\right] + \ldots$$

Bayesian and MAP Estimates

$$p(x|D) = \int p(x|\Theta)\, p(\Theta|D)\, d\Theta = \int \left[p(x|\hat{\Theta}) + \left.\frac{dp(x|\Theta)}{d\Theta}\right|_{\hat{\Theta}} (\Theta - \hat{\Theta}) + \frac{1}{2} \left.\frac{d^2 p(x|\Theta)}{d\Theta^2}\right|_{\hat{\Theta}} (\Theta - \hat{\Theta})^2 + \ldots \right] p(\Theta|D)\, d\Theta$$

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$$= p(x|\hat{\Theta}) + \left.\frac{dp(x|\Theta)}{d\Theta}\right|_{\hat{\Theta}} E\left[(\Theta - \hat{\Theta})|D\right] + \frac{1}{2} \left.\frac{d^2 p(x|\Theta)}{d\Theta^2}\right|_{\hat{\Theta}} E\left[\left(\Theta - \hat{\Theta}\right)^2 |D\right] + \ldots$$

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Handwaving arg: As data increases, the posterior becomes more sharply peaked about the MAP value $\hat{\Theta}$, trailing terms will become small & integral is approximately

$$p(x|D) \approx p(x|\hat{\Theta})$$

Recursive Bayesian Estimation

Back to Bayesian estimation of p(x|D)

$$p(x|D) = \int p(x|\Theta)\, p(\Theta|D)\, d\Theta = \int p(x|\Theta) \frac{p(D|\Theta)\, p(\Theta)}{\int p(D|\Theta')\, p(\Theta')\, d\Theta'}\, d\Theta$$

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Denote the dataset with n points by D^n = {x1, x2, …, xn}, and its likelihood by

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$$p(D^n|\Theta) = \prod_{k=1}^{n} p(x_k|\Theta) = p(x_n|\Theta)\; p(D^{n-1}|\Theta)$$

Using the last expression, the posterior can be written

$$p(\Theta|D^n) = \frac{p(x_n|\Theta)\; p(\Theta|D^{n-1})}{\int p(x_n|\Theta')\; p(\Theta'|D^{n-1})\, d\Theta'}$$

Recursive Bayesian Estimation

We have written the posterior density for the n-sample data set as

$$p(\Theta \mid D^n) = \frac{p(x_n \mid \Theta)\ p(\Theta \mid D^{n-1})}{\int p(x_n \mid \Theta')\ p(\Theta' \mid D^{n-1}) d\Theta'}$$

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Starting with zero data, we take $p(\Theta \mid D^0) = p(\Theta)$ and generate the sequence

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$$p(\Theta \mid D^1),\ p(\Theta \mid D^2),\ \ldots$$

and thus <u>incrementally refine</u> our estimate of the posterior density as more and more data becomes available.

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How Does a Bayesian do Regression?

Get a dataset $D \equiv \{ (x_i, t_i) \; i = 1, \ldots, m \}$

Choose a parameterized regression function f(x;Θ) to fit to the data.

Choose a model distribution function for the targets, e.g. a Gaussian

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$$p(t \mid x, \sigma^2, \Theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2\sigma^2} \left(t - f(x;\Theta) \right)^2 \right]$$

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Choose a prior distribution on the parameters $p(\Theta, \sigma^2)$.

Calculate the data likelihood and the posterior distribution of the parameters

$$p(\Theta, \sigma^2 \mid D) = \frac{1}{p(D)} \; p(D \mid \Theta, \sigma^2) \; p(\Theta, \sigma^2)$$

How Does a Bayesian Do Regression?

Calculate the target density as a function of x by integrating over the posterior distribution of the parameters

$$p(t \mid x, D) \;=\; \int p(t \mid x, \sigma^2, \Theta)\;\; p(\sigma^2, \Theta \mid D)\;\; d\sigma^2 \;\; d\Theta$$

From the distribution on t, we can calculate several quantities.

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- The conditional mean E[t | x,D]) (called the <u>regressor</u>, and equal to

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$$E[t \mid x, D] = \int t \;\; p(t \mid x, D)\, dt$$

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$$= \int t\; p(t \mid x, \sigma^2, \Theta)\; dt\; d\sigma^2\; d\Theta = \int f(x; \Theta)\; p(\Theta \mid D)\, d\Theta$$

  for our Gaussian model.)

- The most likely value(s) of t $\quad \arg\max_t \; p(t \mid x, D)$

- The target variance var(t | x,D).

Hyperparameters and Model Selection

Our prior on model parameters is itself a parameterized distribution. Recall for our Gaussian density model, we put a prior on the distribution of the mean

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$$p(\mu \mid \mu_0, \lambda^2) = \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left[-\frac{1}{2\lambda^2} (\mu - \mu_0)^2 \right]$$

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But how were the <u>hyperparameters chosen</u> $\mu_0, \ \lambda^2$

Hyperparameter Selection

- We could calculate the likelihood function for particular values

$$p(D \mid \mu_0, \lambda^2) = \int p(D \mid \mu) \; p(\mu \mid \mu_0, \lambda^2) \; d\mu$$

and choose the values of the hyperparameters that maximizes it.

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- We could set up a hyperprior on the hyperparameters and choose maximum aposteriori values for the hyperparameters by maximizing

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$$p(\mu_0, \lambda^2 \mid D) \propto p(D \mid \mu_0, \lambda^2) \; p(\mu_0, \lambda^2)$$

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(but the hyperprior is going to have its own parameters …).

- Use some sort of empirical technique.

Empirical Hyperparameter Selection

Using a ‘validation’ set and MAP estimates.
Divide data into two pieces, development and evaluation

Development	Eval.

Further divide the development set into fitting and validation

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$\Lambda 1$	Fitting	Valid.
$\Lambda 2$	Fitting	Valid.
$\Lambda 3$	Fitting	Valid.

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Sweep the hyperparameters over a range $a<\Lambda<b$, and for value, fit the model finding the MAP estimate of the model parameter $\Theta(\Lambda_i,D)$. Measure the performance on the validation set.

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Find the Λ that gives the best performance on the validation set, and use this value to generate a new MAP estimate using the <u>entire</u> dev. set. Test on eval.

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