annotated version

Machine Learning Course - CS-433

Model Selection

Oct 9, 2018

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Last updated: October 9, 2018

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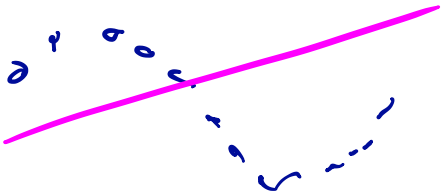
Motivation

We have seen in ridge regression that the regularization parameter $\lambda > 0$ can be tuned to reduce overfitting by reducing model complexity,

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 \quad + \quad \lambda \|\mathbf{w}\|^2$$

The parameter λ is a *hyper-parameter.*



Or: Enrich the model complexity, by augmenting the feature vector $\mathbf{x}$. E.g., polynomial feature expansion. Here the degree d is a hyperparameter.

Neural nets: Tens or hundreds of hyperparameters: architechture, width, depth, type of the network etc.

In all these cases we are faced with the same problem: how do we choose these hyperparameters? This is the *model selection* problem.

Probabilistic Setup

Probabilistic view on the data:

There is an (unknown) underlying distribution $\mathcal{D}$, with range $\mathcal{X} \times \mathcal{Y}$. The data set we see, call it S, consists of independent samples from $\mathcal{D}$:

$$S = \{(\mathbf{x}_n, y_n) \text{ i.i.d.} \sim \mathcal{D}\}_{n=1}^{N}.$$

The *learning algorithm* computes the "best" model within the class of given models. E.g., for ridge regression, with a fixed parameter λ, gives the best $\mathbf{w}$.
Write $f_S = \mathcal{A}(S)$, where $\mathcal{A}$ denotes the learning algorithm, which depends on the data subset S we are given and f_S is the resulting prediction function or model.

If we want to indicate that f_S also depends on parameters of the model, e.g., the λ in the ridge regression model, we can add a subscript to write $f_{S,\lambda}$.

Example

Ridge regression

$f_S(x) = x^T w$

trained on set S

Training Error versus Generalization Error

Given a model f, how can we assess if f is any good? Should compute the *expected* error over all samples chosen according to $\mathcal{D}$,

$$L_{\mathcal{D}}(f) = \mathbb{E}_{\mathcal{D}}[\ell(y, f(\mathbf{x}))],$$

where $\ell(\cdot,\cdot)$ is our loss function. E.g., for ridge regression

$$\ell(y, f(\mathbf{x})) = \tfrac{1}{2}(y - f(\mathbf{x}))^2,$$

The quantity $L_{\mathcal{D}}(f)$ has many names: generalization error, (true/expected) risk, (true/expected) loss. This is the quantity we are fundamentally interested in, but we cannot compute it since $\mathcal{D}$ is not known.

Random Selection of S from $\mathcal{D}$

Example:

$$\ell(y, \tilde{y}) = (y - \tilde{y})^2$$

Finite data set
$|S| = N$

We have given a data subset S. It is therefore natural to compute the equivalent *empirical* quantity

error

$$L_S(f) = \frac{1}{|S|} \sum_{(\mathbf{x}_n, y_n) \in S} \ell(y_n, f(\mathbf{x}_n)). \tag{1}$$

„efficiently" computable !

One of the problems with (1) is that in applications the prediction function f is *itself* a function of the data S. So in fact, we compute the quantity

$f_S(x) = x^T w$ ↑ training on S (w. regularization or not)

$$L_S(f_S) = \frac{1}{|S|} \sum_{(\mathbf{x}_n, y_n) \in S} \ell(y_n, f_S(\mathbf{x}_n)).$$

This is often called the *training error* and we have already discussed in previous lectures that this training error might not be representative of the error we see on "fresh" samples. The reason that $L_S(f_S)$ might not be close to $L_{\mathcal{D}}(f_S)$ is of course overfitting

$L_S(f_S) = 0$

Splitting the data

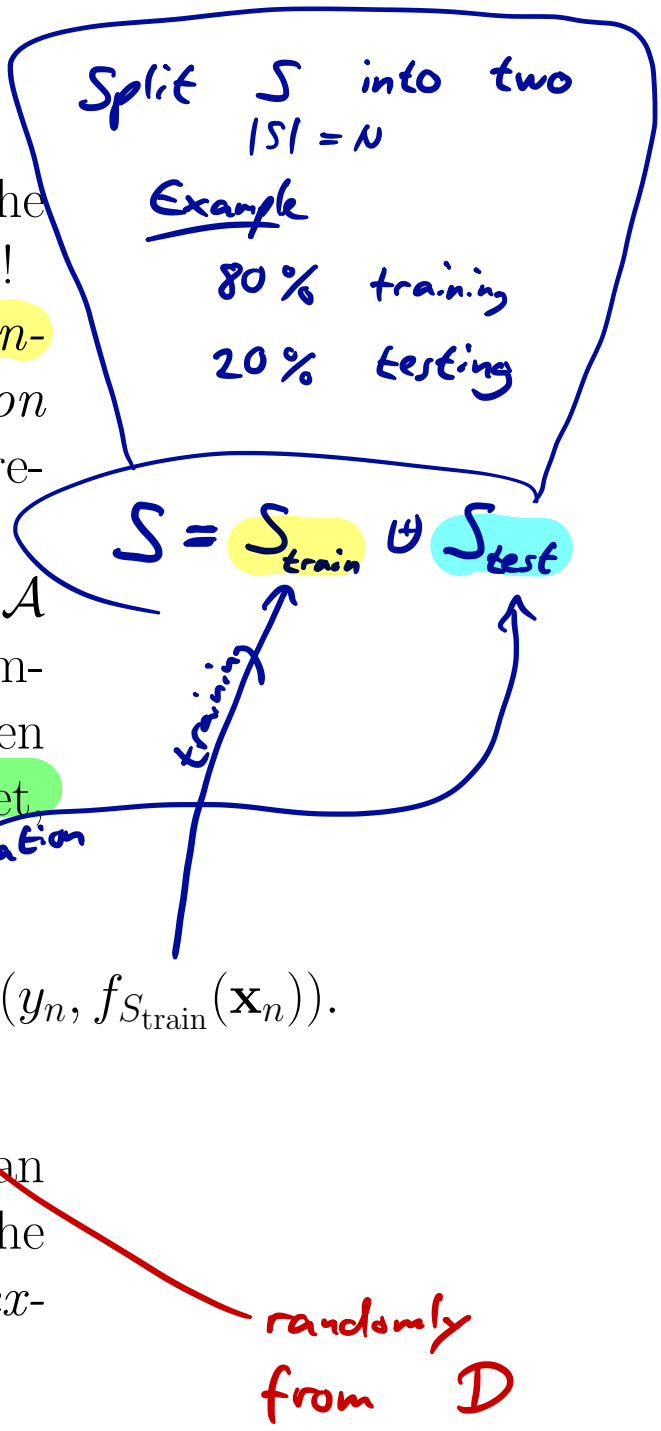
Problem: Validating model on the same data subset we trained it on!
Fix: Split the data into a *training* and a *test* set (a.k.a. *validation* set), call them S_{train} and S_{test}, respectively.
We apply the learning algorithm $\mathcal{A}$ to the training set S_{train} and compute the function $f_{S_{\text{train}}}$. We then compute the error on the test set, i.e.,

$$L_{S_{\text{test}}}(f_{S_{\text{train}}}) = \frac{1}{|S_{\text{test}}|} \sum_{(y_n, \mathbf{x}_n) \in S_{\text{test}}} \ell(y_n, f_{S_{\text{train}}}(\mathbf{x}_n)).$$

Since S_{test} is a "fresh" sample we can hope that $L_{S_{\text{test}}}(f_{S_{\text{train}}})$ is close to the quantity $L_{\mathcal{D}}(f_{S_{\text{train}}})$. Indeed, in *expectation* both are the same, i.e.,

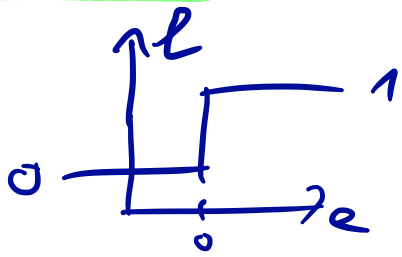
$$L_{\mathcal{D}}(f_{S_{\text{train}}}) = \mathbb{E}_{S_{\text{test}} \sim \mathcal{D}}[L_{S_{\text{test}}}(f_{S_{\text{train}}})], \tag{2}$$

where the expectation is over the samples of the test set. (For a particular test set S_{test} they might differ due to the randomness from the selection of the test set.)



But we payed a price. We had to split the data and now have less data both for the learning as well as the validation (test) task.
"Cross validation" as described below is more efficient in using data, but hard to analyze.

Generalization Error versus Test Error



Assume that we have a model f, and that our loss function $\ell(\cdot,\cdot)$ is bounded, lets say in $[a,b]$. We are given a test set S_{test} chosen i.i.d. from the underlying distribution $\mathcal{D}$. The test error (empirical error) is

$$L_{S_{\text{test}}}(f) = \frac{1}{|S_{\text{test}}|} \sum_{(\mathbf{x}_n,y_n)\in S_{\text{test}}} \ell(y_n, f(\mathbf{x}_n)).$$

The true generalization error is

$$L_{\mathcal{D}}(f) = \mathbb{E}_{(y,\mathbf{x})\sim\mathcal{D}}[\ell(y, f(\mathbf{x}))].$$

How far are these apart? We have seen in (2) that in expectation they are the same. But we need to worry about the variation. We claim that

quality parameter $\delta > 0$

$$\mathbb{P}\Big[\,\big|L_{\mathcal{D}}(f) - L_{S_{\text{test}}}(f)\big| \geq \sqrt{\frac{(b-a)^2\ln(2/\delta)}{2|S_{\text{test}}|}}\,\Big] \leq \delta. \quad (3)$$

proof idea

$$\mathbb{P}\big[\ \ldots \geq \varepsilon\ \big] \leq e^{\ldots\varepsilon^2\ldots}$$

Insights: Error decreases as $\mathcal{O}(1/\sqrt{|S_{\text{test}}|})$ with the number test points. The more data points we have therefore, the more confident we can be that the empirical loss we measure is close to the true loss.

Proof of (3):
Since we assumed that each data sample $(\mathbf{x}_n, y_n)$ in the test set S_{test} is chosen independently, the associated losses $\ell(y_n, f(\mathbf{x}_n))$, given a fixed model f, are also i.i.d. random variables, taking values in $[a, b]$ by assumption. Call each such loss Θ_n. The expected value of $\Theta_n = \ell(y_n, f(\mathbf{x}_n))$ is equal to the true loss

$$L_{\mathcal{D}}(f) = \mathbb{E}[\ell(y_n, f(\mathbf{x}_n))].$$

The empirical loss on the other hand is equal to the average of $|S_{\text{test}}|$ such i.i.d. values.
We want to know the chance that the empirical loss $L_{S_{\text{test}}}(f))$ deviates from its true value by more than a given constant. This is a classical problem addressed in the following lemma.

Lemma 0.1 (Chernoff Bound). *Let $\Theta_1, \ldots, \Theta_N$ be a sequence of i.i.d. random variables with mean $\mathbb{E}[\Theta]$ and range $[a, b]$. Then, for any $\varepsilon > 0$,*

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{n=1}^{N}\Theta_n - \mathbb{E}[\Theta]\right| \geq \varepsilon\right] \leq 2e^{-2N\varepsilon^2/(b-a)^2}$$

Using Lemma 0.1 let us show (3). Equating $2e^{-2|S_{\text{test}}|\varepsilon^2/(b-a)^2}$ with δ we get that $\varepsilon = \sqrt{\frac{(b-a)^2 \ln(2/\delta)}{2|S_{\text{test}}|}}$ as claimed.

set $\delta :=$

solve for ε

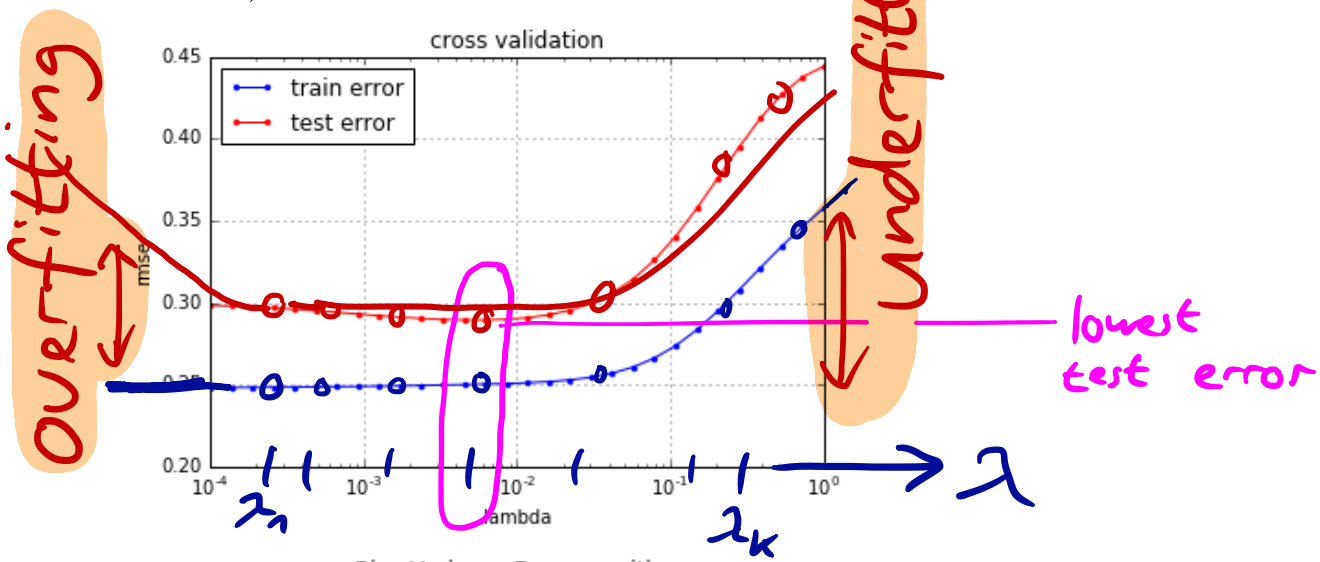
Model selection

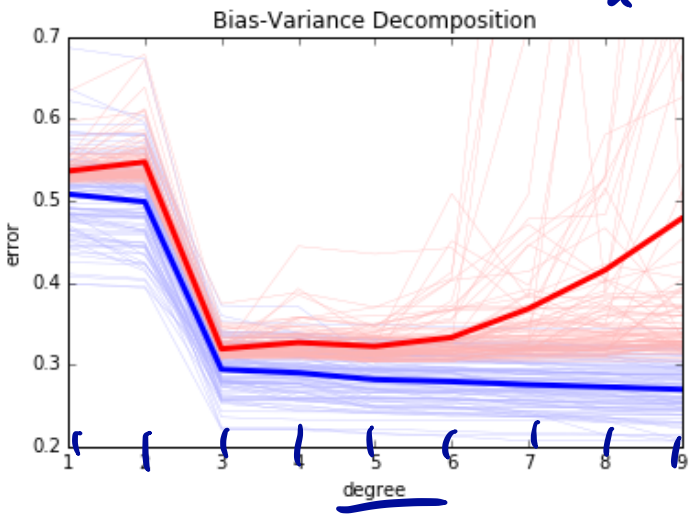
Let us summarize our main goal: We are looking for a way to select the hyperparameters of our model, like the parameter λ for the ridge regression problem. We split our data into one training set S_{train} and one test set S_{test} and we think of them as having been generated independently and sampled according to the underlying but unknown distribution $\mathcal{D}$. We have in addition a set of values for a parameter of the model, e.g., the parameter λ in the ridge regression problem. Let these values be λ_k, $k = 1, \ldots, K$. To keep things simple we assume that K is some finite value.

We run the learning algorithm K times on the same training set S_{train} to compute the K prediction functions $f_{S_{\text{train}},\lambda_k}$. For each such prediction function we compute the test error $L_{S_{\text{test}}}(f_{S_{\text{train}},\lambda_k})$. We then choose that value of the parameter λ which gives us the smallest such test error.

In the figure below, we plot the test error (red) as well as the training error (blue) for many values of λ (grid search).

$\|Xw - y\|^2 + \lambda\|w\|^2$





another hyperparam

Does model selection work? Using now separate data sets for training and test we are still faced with several questions.

The first question concerns the learning. How do we know that the function $f_{S_{\text{train}},\lambda}$ is a good approximation of the function $f_{\mathcal{D}}$, the best model within our class for the underlying distribution? We will discuss this issue in our next lecture.

The second question concerns the validation/test: How do we know that, for a fixed function f, $L_{S_{\text{test}}}(f)$ is a good approximation to $L_{\mathcal{D}}(f)$? In other words, how do we know that the empirical error is close to the true error? Let us discuss this issue next.

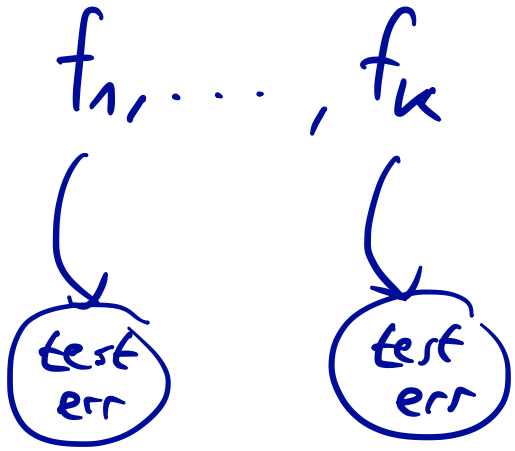
$f_{S_{train}} \overset{?}{\approx} f_{best}$

$L_{S_{test}}(f) \overset{?}{\approx} L_{\mathcal{D}}(f)$

answered before for the case of a single model

Model Selection Based on Test Error

Follow "*Generalization Error versus Test Error*", but now we have K models f_k given as candidates, $k = 1, \ldots, K$. Again assume our loss function $\ell(\cdot, \cdot)$ is bounded in $[a, b]$. Given a test set S_{test} chosen i.i.d. from $\mathcal{D}$.



How far is each of the K test errors (empirical errors) $L_{S_{\text{test}}}(f_k)$ from the true $L_{\mathcal{D}}(f_k)$?

Similarly as in the case of a single model (3), we claim that we can now bound the deviation for all k candidates, by

all models are close to their true error

$$\mathbb{P}\left[\max_k \left| L_{\mathcal{D}}(f_k) - L_{S_{\text{test}}}(f_k) \right| \geq \sqrt{\frac{(b-a)^2 \ln(2K/\delta)}{2|S_{\text{test}}|}} \right] \leq \delta. \tag{4}$$

Insights: Error decreases as $\mathcal{O}(1/\sqrt{|S_{\text{test}}|})$ with the number test points. Now that we test K hyper-parameters, our error only goes up by a very small factor which is proportional to $\sqrt{\ln(K)}$. So we can test many different models without incurring a large penalty.

The proof of this statement follows (3), which has answered the special case of $K = 1$.

For a general K, if we check the deviations for K independent samples and ask for the probability that for at least one such sample we get a deviation of at least ε then by the union bound this probability is at most K times as large as in the case where we are only concerned with a single instance. I.e., the upper bound becomes $2Ke^{-2|S_{\text{test}}|\varepsilon^2/(b-a)^2}$.

Hence, equating now $2Ke^{-2|S_{\text{test}}|\varepsilon^2/(b-a)^2}$ with δ we get that $\varepsilon = \sqrt{\frac{(b-a)^2 \ln(2K/\delta)}{2|S_{\text{test}}|}}$ as stated.

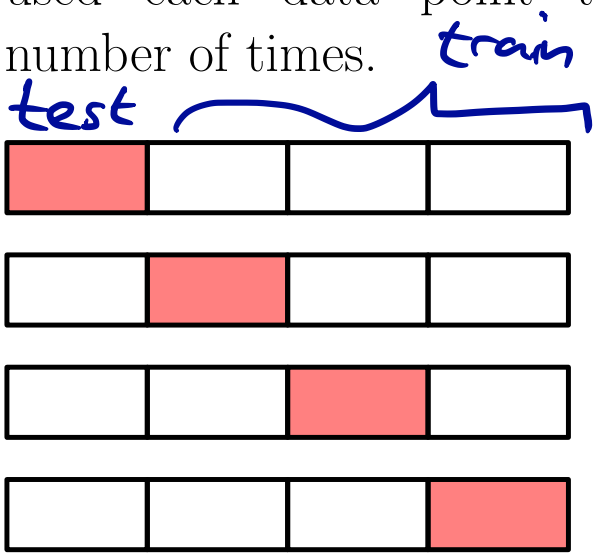
Extension to infinitely many model choices. The basic idea of this bound can be carried over to the case where we have infinitely many models. In this case a more sophisticated concept, called the VC-dimension, is used: as long as we have models with a *finite* VC-dimension then the bound one can show has the same form, with K replaced by the VC dimension.

Cross-validation

Splitting the data once into two parts (one for training and one for testing) is not the most efficient way to use the data. Cross-validation is a better way:

K-fold cross-validation is a popular variant. Randomly partition the data into K groups. Now train K times. Each time leave out exactly one of the K groups for testing and use the remaining $K-1$ groups for training. Average the K results.

Note: Have used all data for training, and all data for testing, and used each data point the same number of times.



Cross-validation returns an unbiased estimate of the *generalization error* and its variance.

Do this for every choice of hyper-param.

we will use the average of

- test error

sometimes also

- training error
- model weights w

over the K folds

Additional Notes

Proof of Lemma 0.1

Instead of considering the setup in the lemma we can equivalently assume that $\mathbb{E}[\Theta] = 0$ and that the Θ_n take values in $[a, b]$, where $a \leq 0 \leq b$. We will show that

$$\mathbb{P}\{\frac{1}{N}\sum_{n=1}^{N}\Theta_n \geq \varepsilon\} \leq e^{-2N\varepsilon^2/(b-a)^2}.$$

This, together with the equivalent bound

$$\mathbb{P}\{\frac{1}{N}\sum_{n=1}^{N}\Theta_n \leq -\varepsilon\} \leq e^{-2N\varepsilon^2}$$

will prove the claim. We have

$$\begin{aligned}
\mathbb{P}\{\frac{1}{N}\sum_{n=1}^{N}\Theta_n \geq \varepsilon\} &\overset{s>0}{=} \mathbb{P}\{e^{s\frac{1}{N}\sum_{n=1}^{N}\Theta_n} \geq e^{s\varepsilon}\} \\
&\overset{(a)}{\leq} \min_{s>0}\mathbb{E}[e^{s\frac{1}{N}\sum_{n=1}^{N}\Theta_n}]e^{-s\varepsilon} \\
&\overset{(b)}{=} \min_{s>0}\prod_{n=1}^{N}\mathbb{E}[e^{\frac{s\Theta_n}{N}}]e^{-s\varepsilon} \\
&= \min_{s>0}\mathbb{E}[e^{\frac{s\Theta}{N}}]^N e^{-s\varepsilon} \\
&\overset{(c)}{\leq} \min_{s>0} e^{s^2(b-a)^2/(8N)} e^{-s\varepsilon} \\
&\overset{s=4N\varepsilon/(b-a)^2}{=} e^{-2N\varepsilon^2/(b-a)^2}.
\end{aligned}$$

Here, step (a) follows from the Markov inequality. In step (b) we have used the fact that the random variables Θ_n, and

hence the random variables $e^{\frac{s\Theta_n}{N}}$, are independent so that the expectation of the product is equal to the product of the expectations. Finally, in step (c) we have used the so-called Hoeffding lemma. It states that for any random variable X, with $\mathbb{E}[X] = 0$ and $X \in [a, b]$ we have

$$\mathbb{E}[e^{sX}] \leq e^{\frac{1}{8}s^2(b-a)^2}.$$

To give a rough outline, consider the convex function e^{sx}, $s \geq 0$. In the range $[a, b]$ it is upper bounded by the chord (the line that is equal to the function at the two boundaries)

$$e^{sx} \leq \frac{x-a}{b-a}e^{sb} + \frac{b-x}{b-a}e^{sa}.$$

If we now take the expectation with respect to X and recall that $\mathbb{E}[X] = 0$ by assumption then we get

$$\mathbb{E}[e^{sX}] \leq \frac{b}{b-a}e^{sa} - \frac{a}{b-a}e^{sb} \leq e^{s^2(b-a)^2/8}.$$

The last step on the right requires several steps but this is now a pure calculus problem and we skip the details.