Applied Machine Learning

Regularization

Siamak Ravanbakhsh

COMP 551 **(winter 2020)**

Learning objectives

Basic idea of

- overfitting and underfitting
- Regularization (L1 & L2)
- MLE vs MAP estimation
- bias and variance trade off
- evaluation metrics & cross validation

Previously...

Linear regression and logistic regression

is linear too simple? what if it's not a good fit?

how to increase the models expressiveness?

- create new nonlinear features
- is there a downside?

Recall: nonlinear basis functions

replace original features in $f_w(x) = \sum_d w_d x_d$

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linear least squares solution $w^* = (\Phi^\top \Phi)^{-1} \Phi^\top y$

replacing X with Φ

$$\Phi = \begin{bmatrix} \phi_1(x^{(1)}), & \phi_2(x^{(1)}), & \cdots, & \phi_D(x^{(1)}) \\ \phi_1(x^{(2)}), & \phi_2(x^{(2)}), & \cdots, & \phi_D(x^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x^{(N)}), & \phi_2(x^{(N)}), & \cdots, & \phi_D(x^{(N)}) \end{bmatrix}$$

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replacing X with Φ

a (nonlinear) feature

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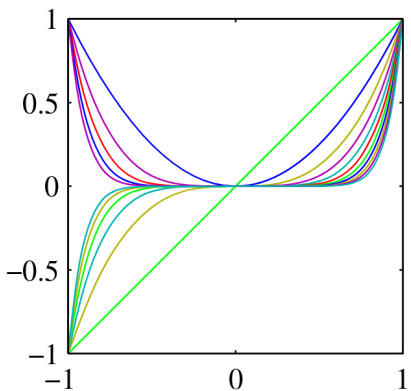
one instance

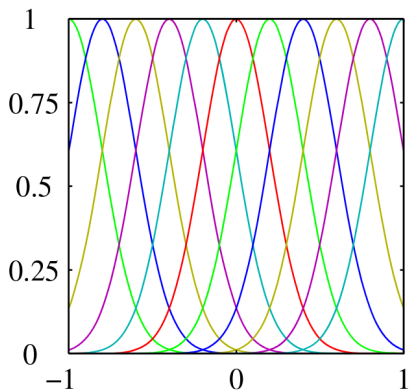
Recall: nonlinear basis functions

examples original input is scalar $x \in \mathbb{R}$



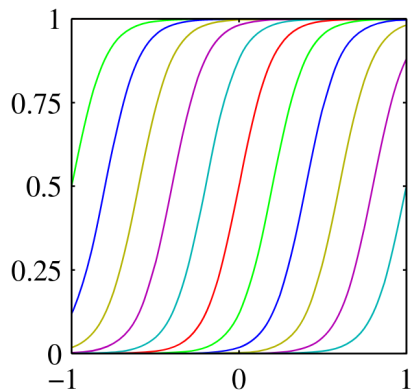
polynomial bases

$$\phi_k(x) = x^k$$



Gaussian bases

$$\phi_k(x) = e^{-\frac{(x-\mu_k)^2}{s^2}}$$



Sigmoid bases

$$\phi_k(x) = \frac{1}{1+e^{-\frac{x-\mu_k}{s}}}$$

Example: Gaussian bases

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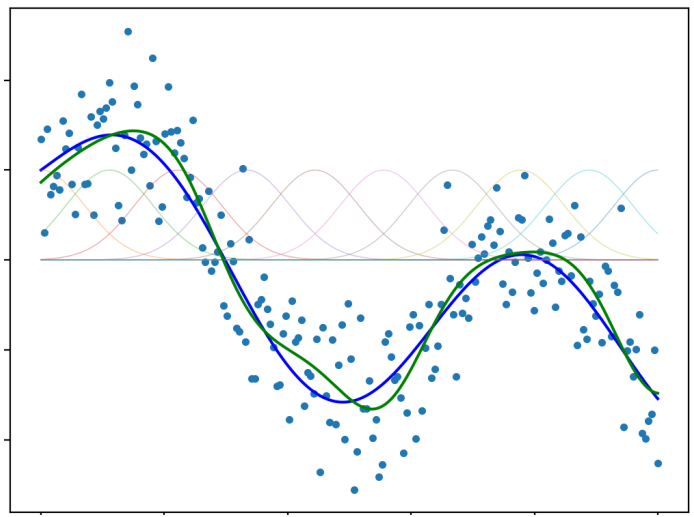

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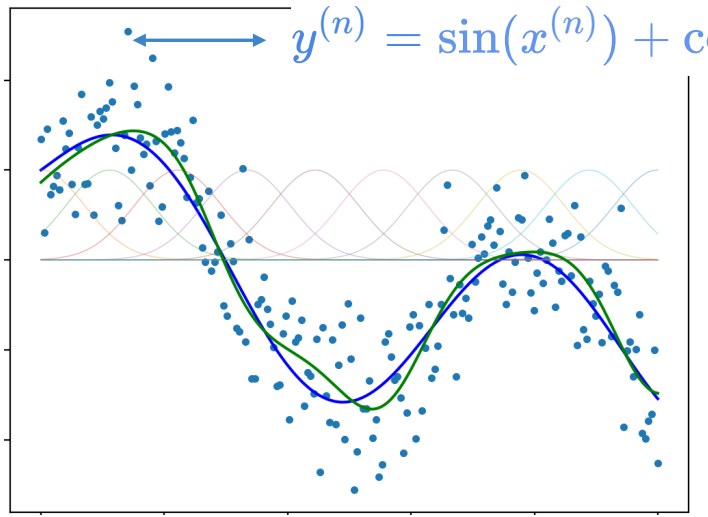

$$y^{(n)} = \sin(x^{(n)}) + \cos(\sqrt{|x^{(n)}|}) + \epsilon$$

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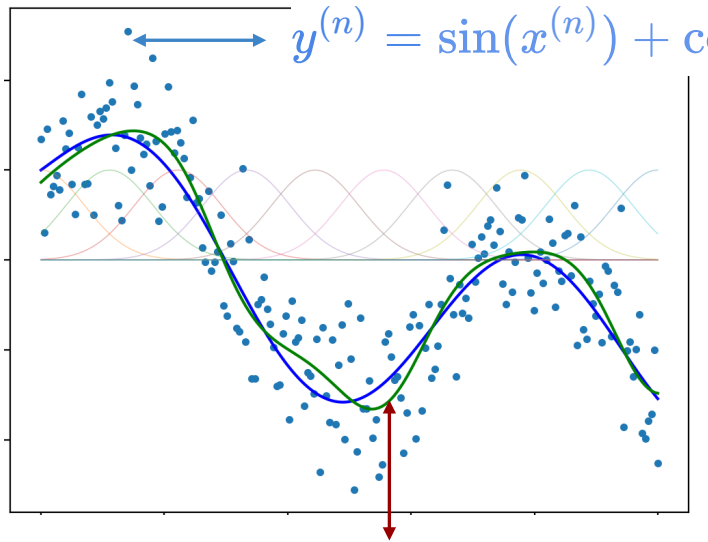

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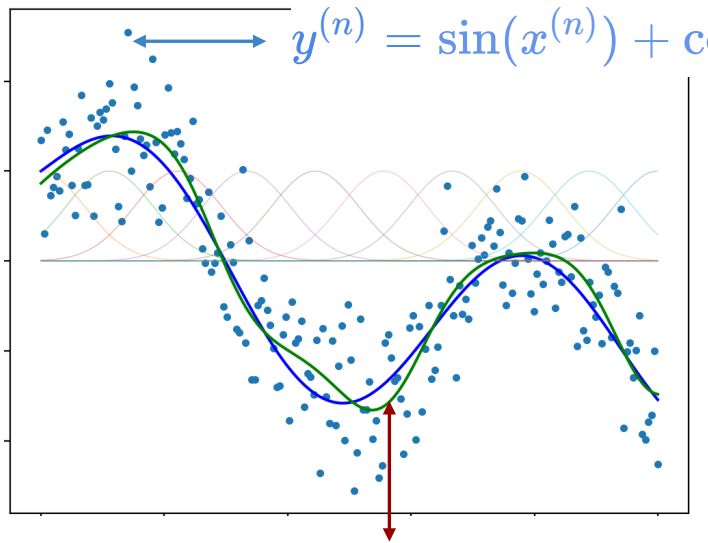

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our fit to data using 10 Gaussian bases

prediction for a new instance

$$f(x') = \phi(x')^\top (\Phi^\top \Phi)^{-1} \Phi^\top y$$

x': new instance

$\phi(x')$: features evaluated for the new point

w found using LLS

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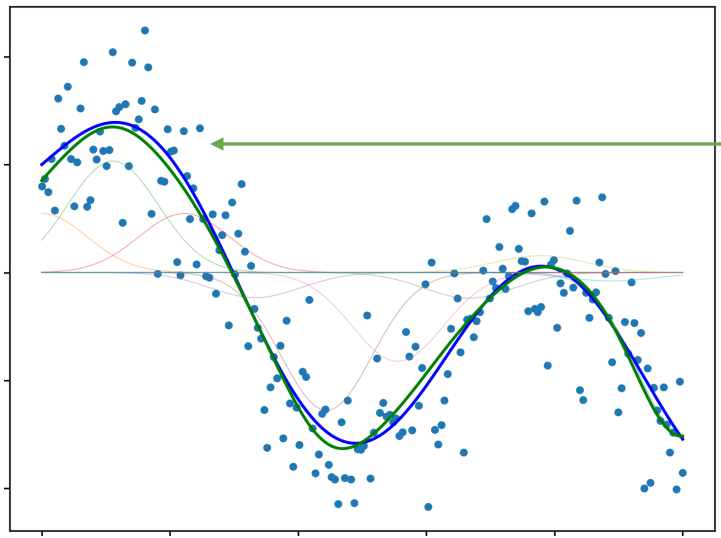


our fit to data using **10 Gaussian bases**

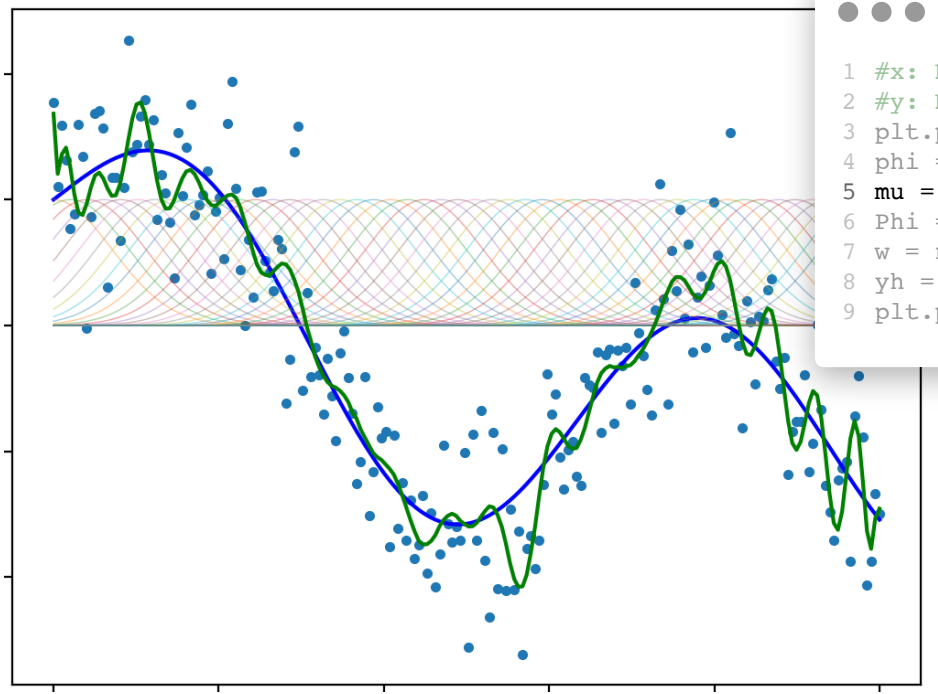
why not more?

```
#x: N
#y: N
plt.plot(x, y, 'b.')
phi = lambda x,mu: np.exp(-(x-mu)**2)
mu = np.linspace(0,10,10) #10 Gaussians bases
Phi = phi(x[:,None], mu[None,:]) #N x 10
w = np.linalg.lstsq(Phi, y)[0]
yh = np.dot(Phi,w)
plt.plot(x, yh, 'g-')
```

Example: Gaussian bases

$$\phi_k(x) = e^{-\frac{(x-\mu_k)^2}{s^2}}$$

using 50 bases



```
#x: N
#y: N
plt.plot(x, y, 'b.')
phi = lambda x,mu: np.exp(-(x-mu)**2)
mu = np.linspace(0,10,50) #50 Gaussians bases
Phi = phi(x[:,None], mu[None,:]) #N x 10
w = np.linalg.lstsq(Phi, y)[0]
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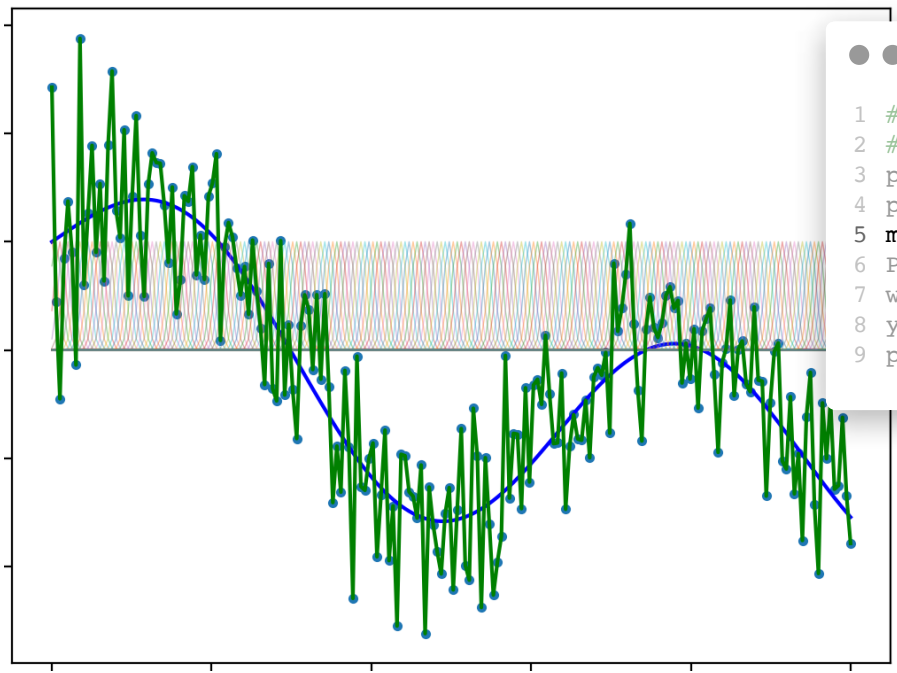
using 200, thinner bases (s=.1)



```
#x: N
#y: N
plt.plot(x, y, 'b.')
phi = lambda x,mu: np.exp(-((x-mu)/.1**2)
mu = np.linspace(0,10,200) #200 Gaussians bases
Phi = phi(x[:,None], mu[None,:]) #N x 10
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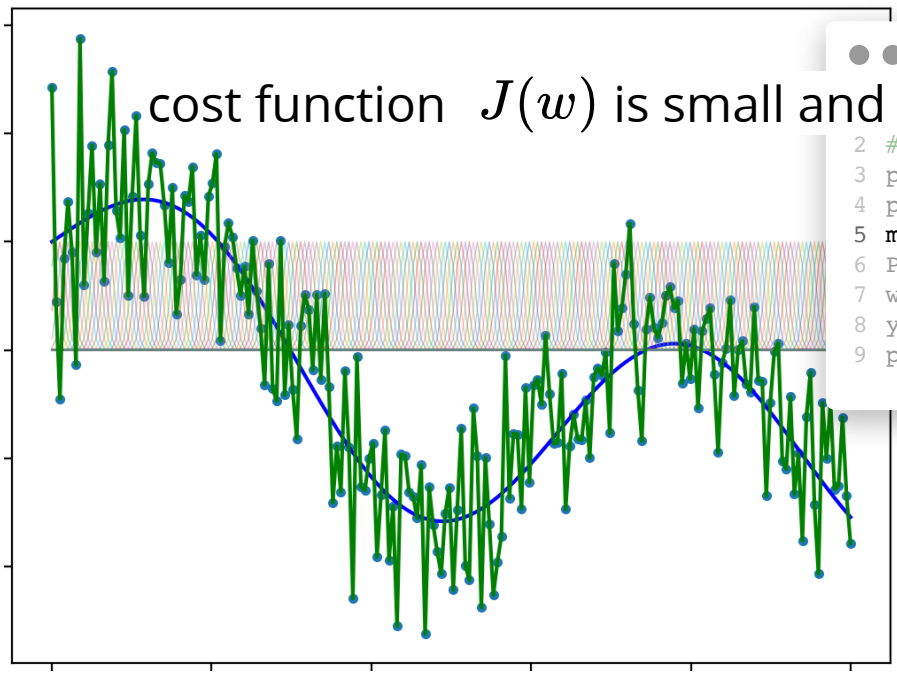

cost function $J(w)$ is small and we have a "*perfect*" fit!

```
#y: N
plt.plot(x, y, 'b.')
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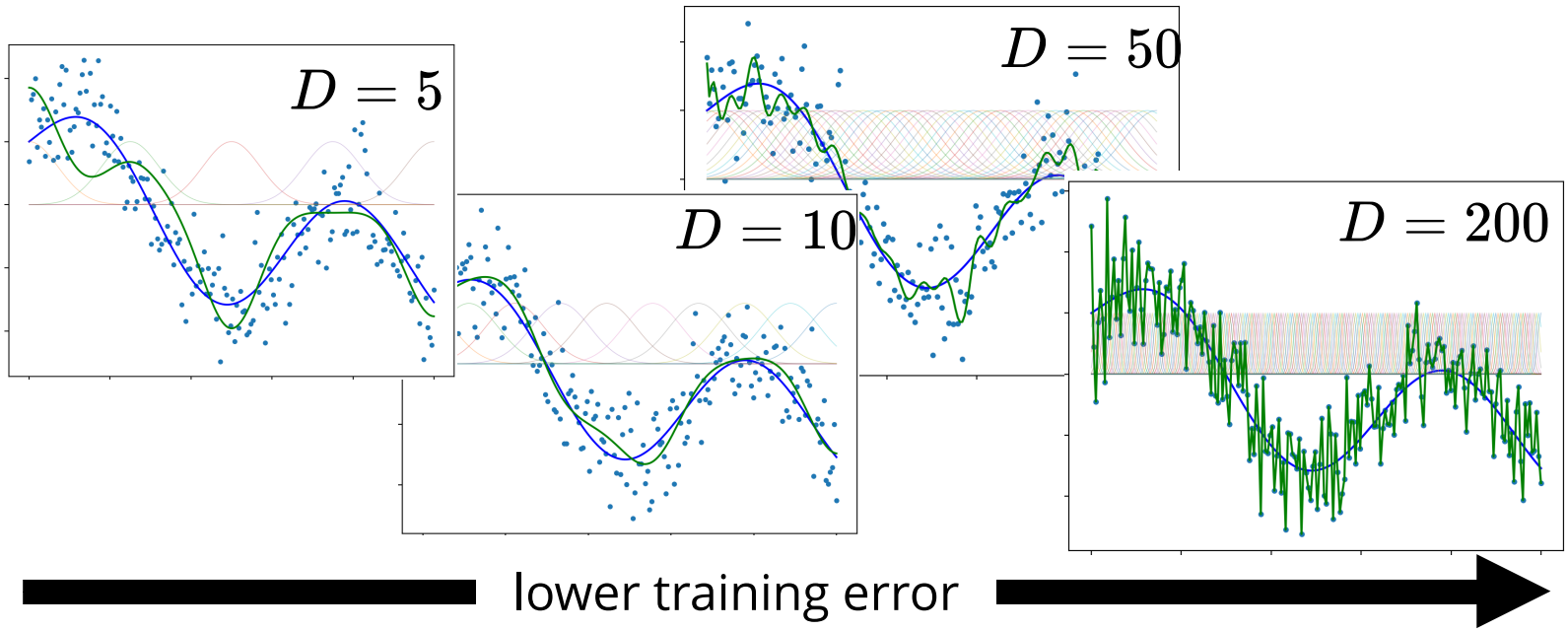
Generalization



which one of these models performs better at test time?

Overfitting

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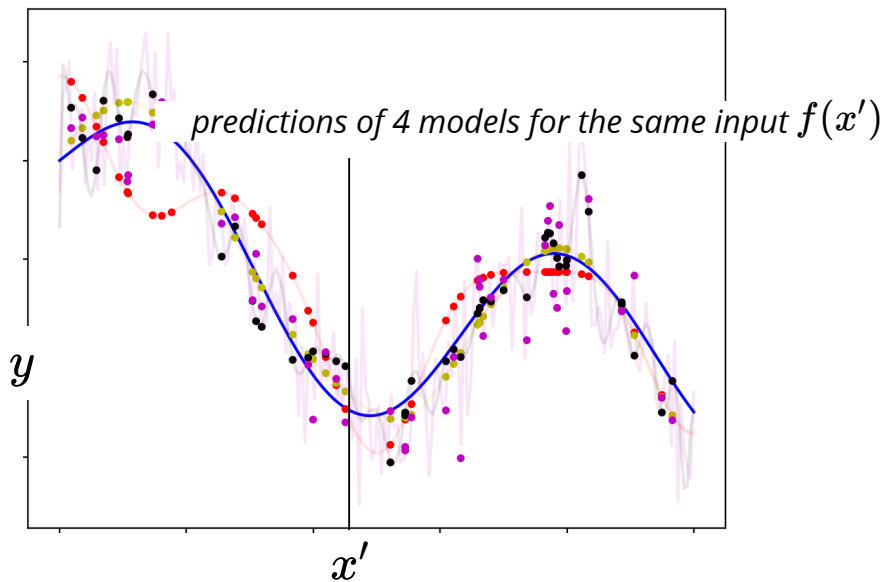

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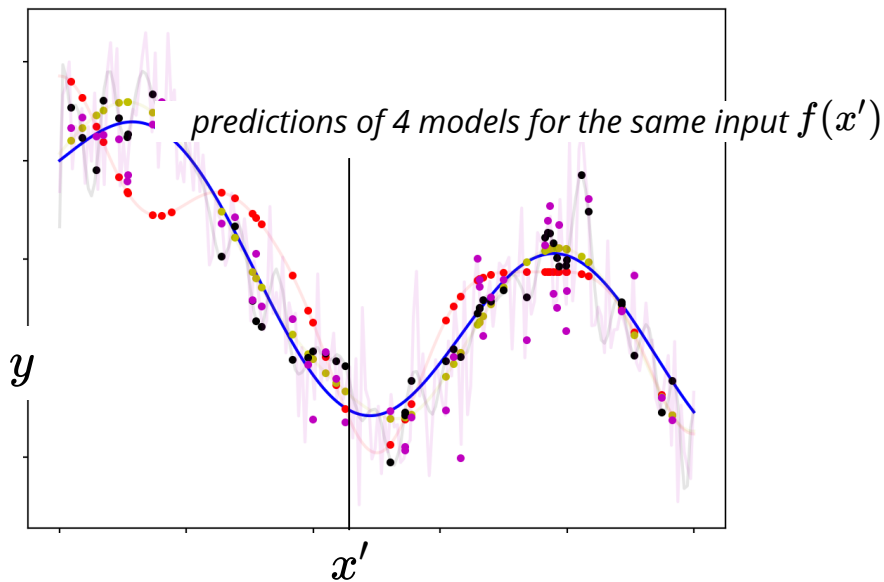

$D = 5$

$D = 10$

$D = 50$

$D = 200$

Overfitting

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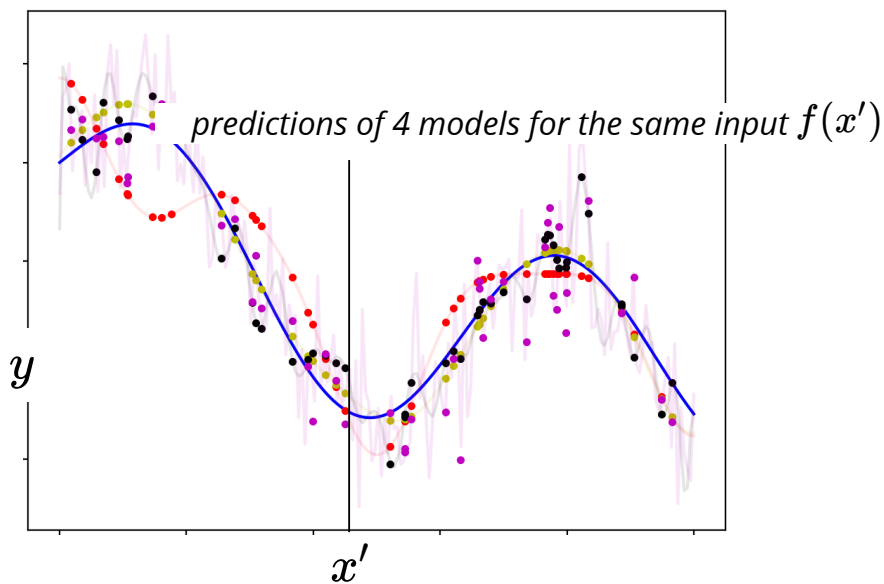

$D = 5$ underfitting

$D = 10$ lowest test error

$D = 50$

$D = 200$ overfitting

Model selection

how to pick the model with lowest expected loss / test error?

regularization bound the test error by bounding

- training error
- model complexity

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when overfitting, we often see large weights

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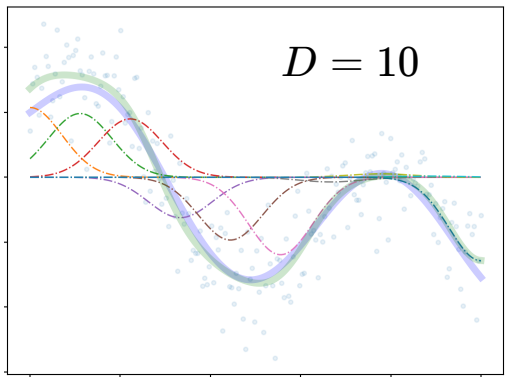

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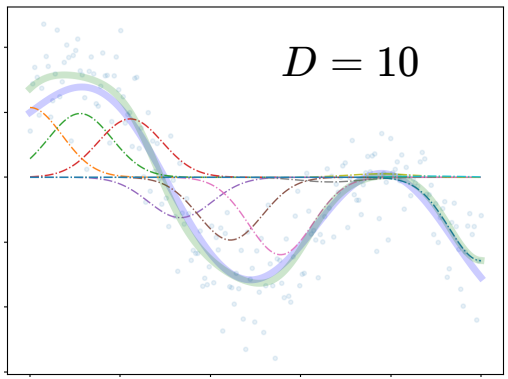

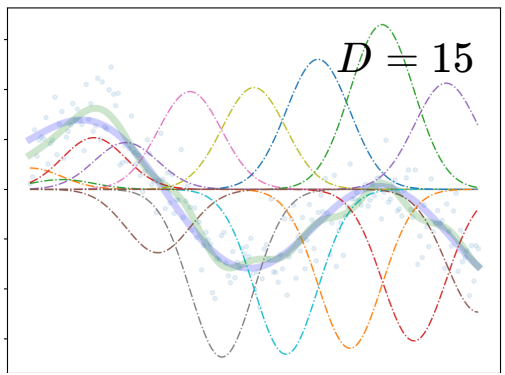

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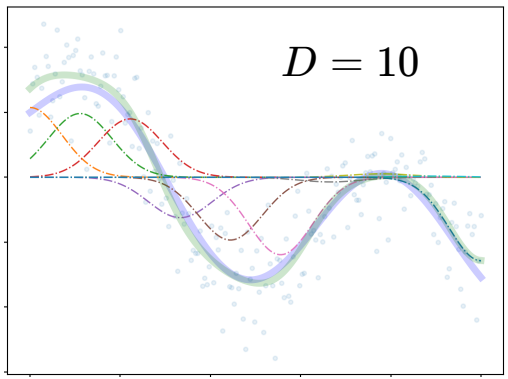

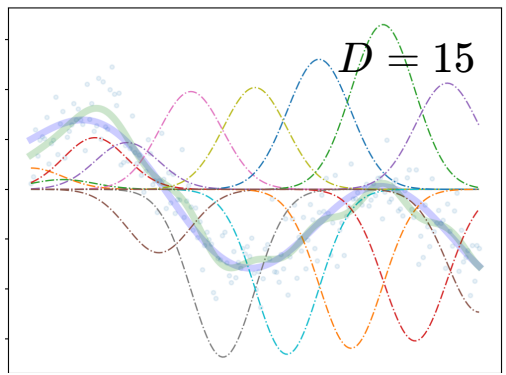

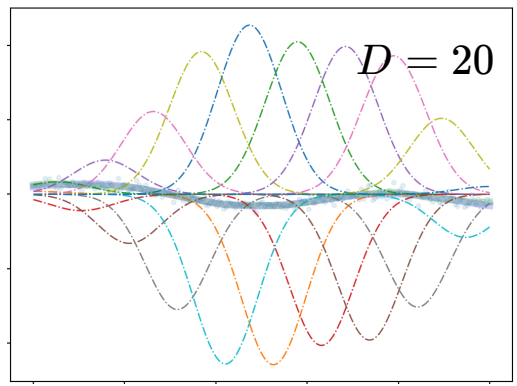

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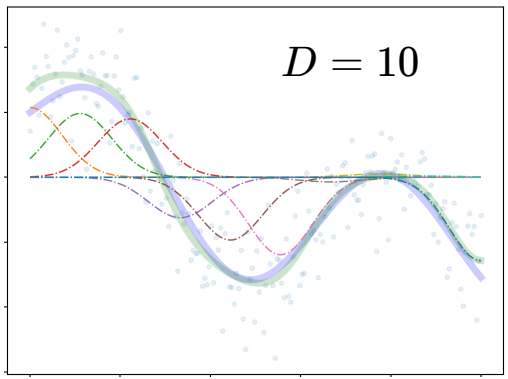

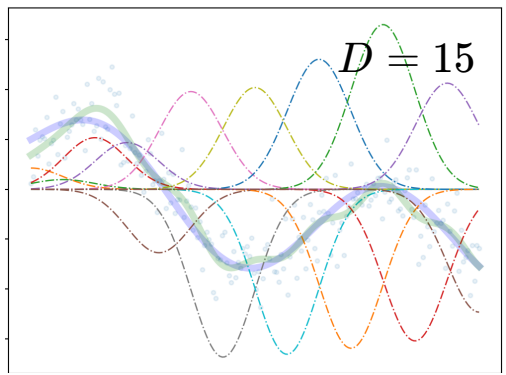

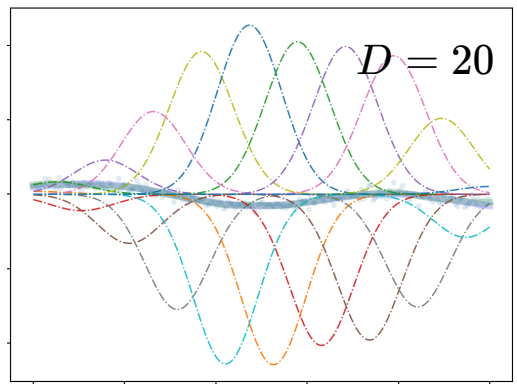

idea: penalize large parameter values

Ridge regression

L2 regularized linear least squares regression:

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a good practice is to not penalize the intercept $\lambda(||w||_2^2 - w_0^2)$

Ridge regression

we can set the derivative to zero

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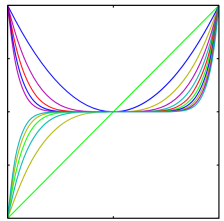
λI makes it invertible!

we can have linearly dependent features (e.g., D > N)

the solution will be unique!

Example: polynomial bases



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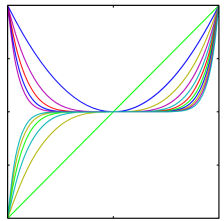

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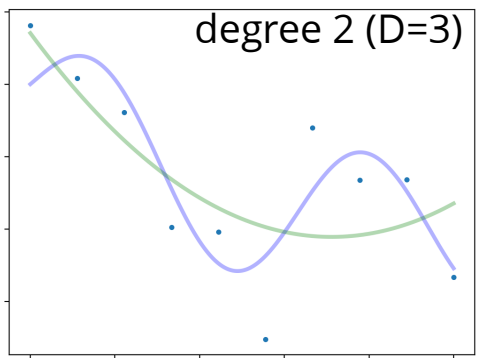

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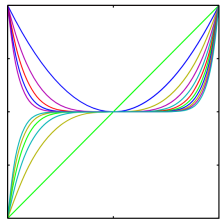

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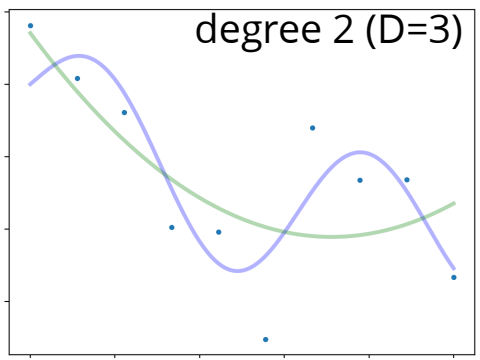

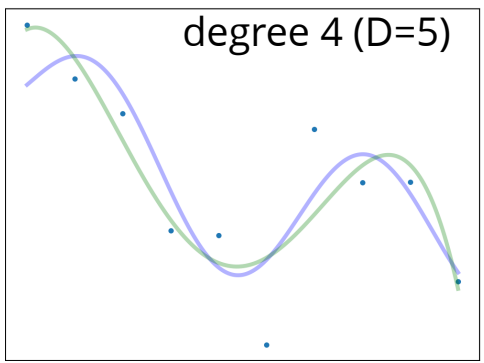

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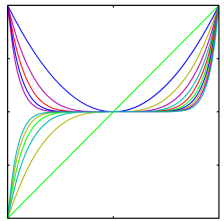

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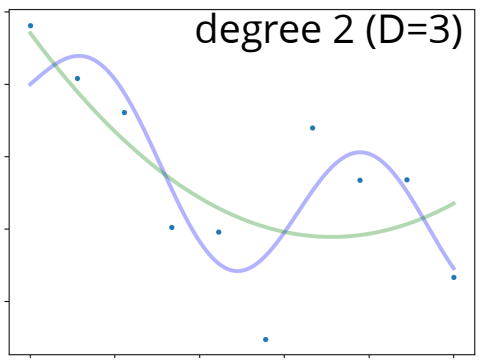
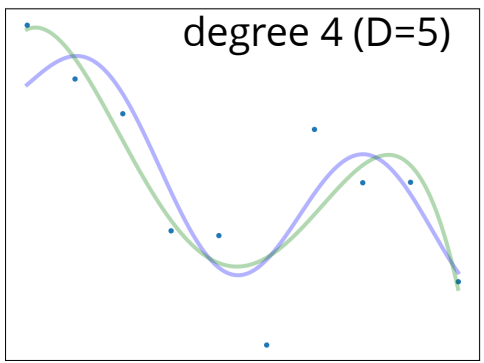
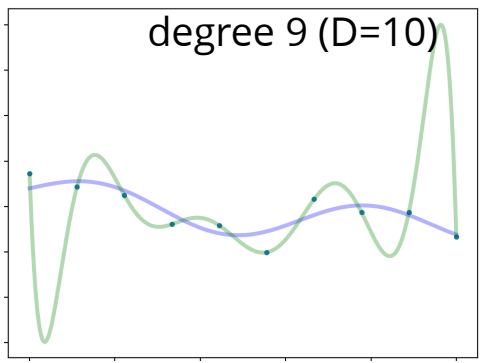
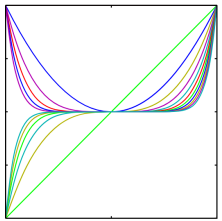






Example: polynomial bases



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$$\phi_k(x) = x^k$$

with regularization:

- fixed D=10, changing the amount of regularization

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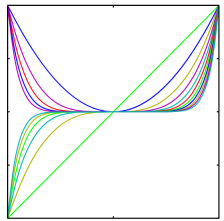

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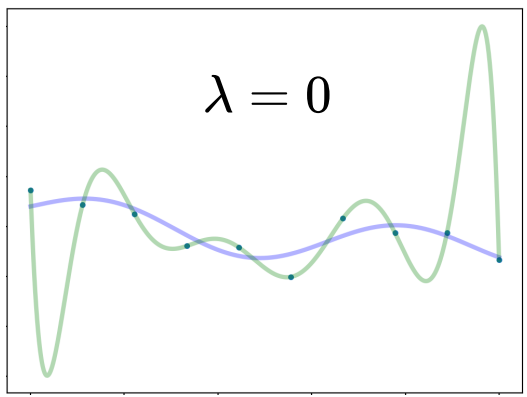

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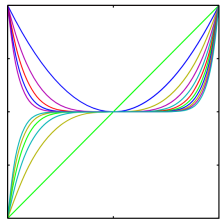

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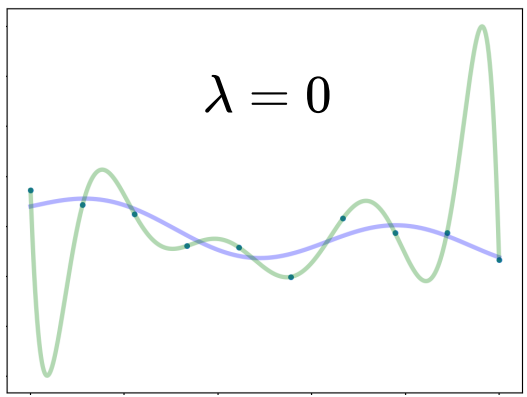

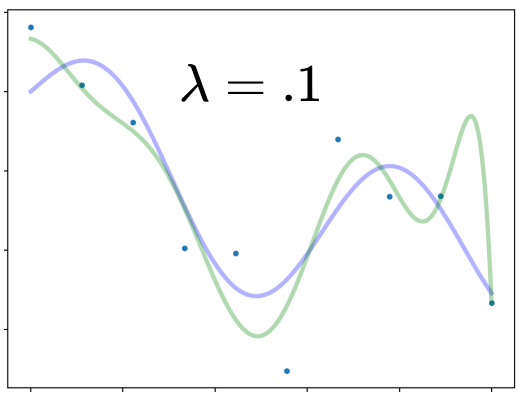

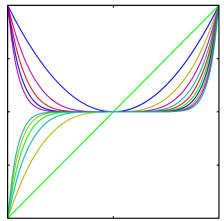

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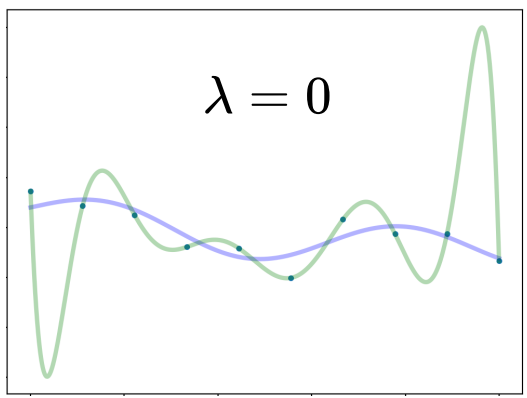

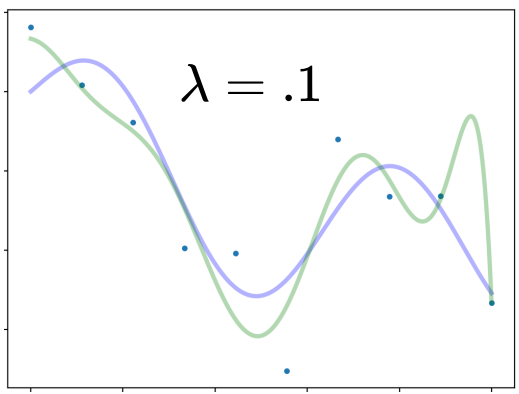

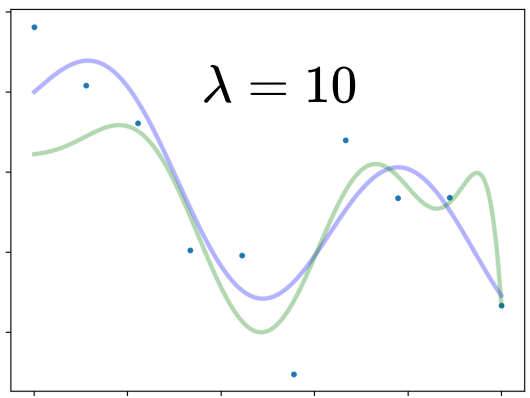

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features of different mean and variance will be penalized differently

normalization

$$\begin{cases} \mu_d = \frac{1}{N} x_d^{(n)} \\ \sigma_d^2 = \frac{1}{N-1} (x_d^{(n)} - \mu_d)^2 \end{cases}$$

makes sure all features have the same mean and variance $x_d^{(n)} \leftarrow \frac{x_d^{(n)} - \mu_d}{\sigma_d}$

Maximum likelihood

previously: linear regression & logistic regression maximize log-likelihood

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linear regression

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idea: maximize the posterior instead of likelihood

$$p(w|y) = \frac{p(w)p(y|w)}{p(y)}$$

Maximum a Posteriori (MAP)

use the Bayes rule and find the parameters with max posterior prob.

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even better would be to estimate the posterior distribution $p(w|y)$

- more on this later in the course!

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Gaussian likelihood and **Gaussian** prior

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multiple data-points

$$\equiv \arg\min_w \tfrac{1}{2} \sum_n (y^{(n)} - w^\top x^{(n)})^2 + \sum_{d=1}^{D} \tfrac{\lambda}{2} w_d^2$$

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L2 regularization

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L2 regularization

L2- regularization is assuming a Gaussian prior on weights

the same is true for logistic regression (or any other cost function)

Laplace prior

another notable choice of prior is the Laplace distribution

image:https://stats.stackexchange.com/questions/177210/why-is-laplace-prior-producing-sparse-solutions

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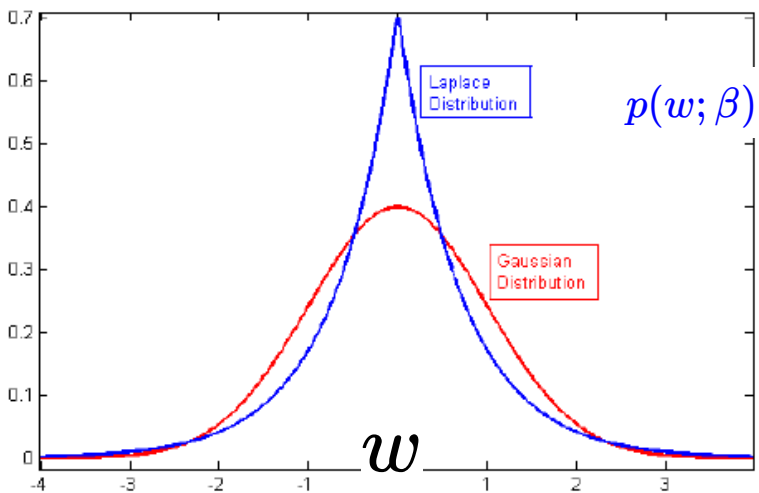

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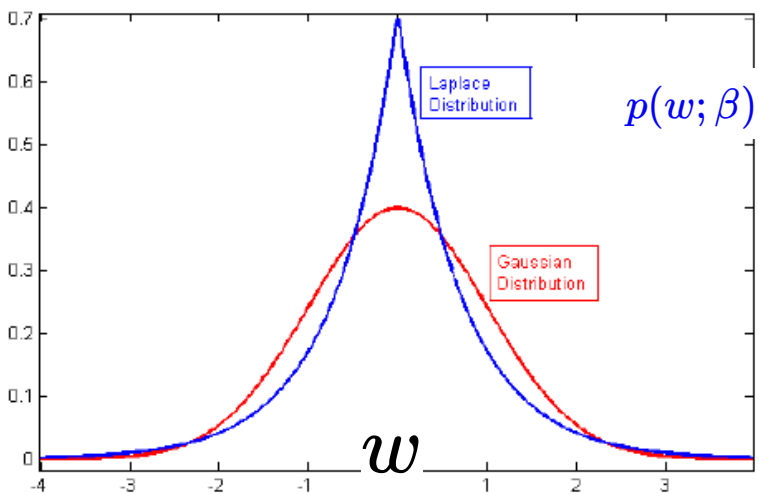

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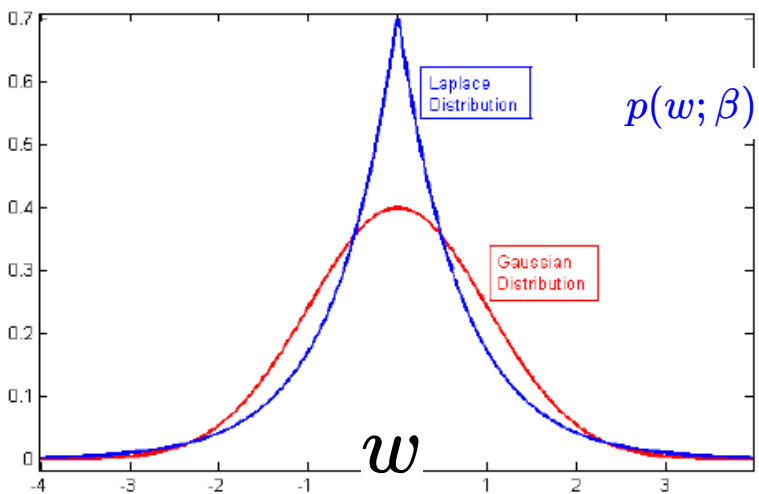

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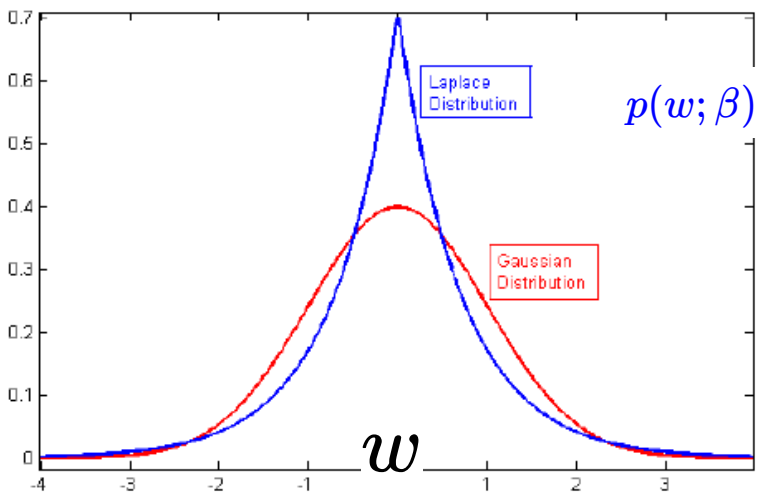
L1 norm of w

L1 regularization: $J(w) \leftarrow J(w) + \lambda||w||_1$ also called lasso

(least absolute shrinkage and selection operator)



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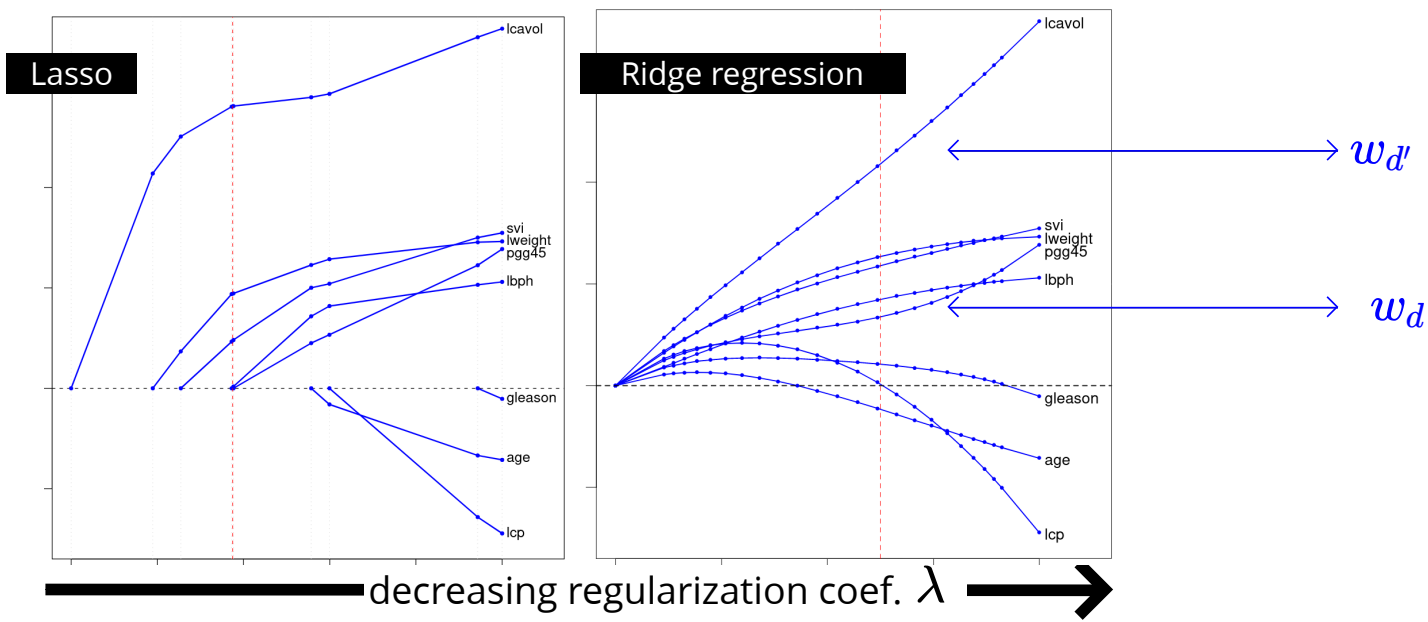
L_1 vs L_2 regularization

regularization path shows how $\{w_d\}$ change as we change λ



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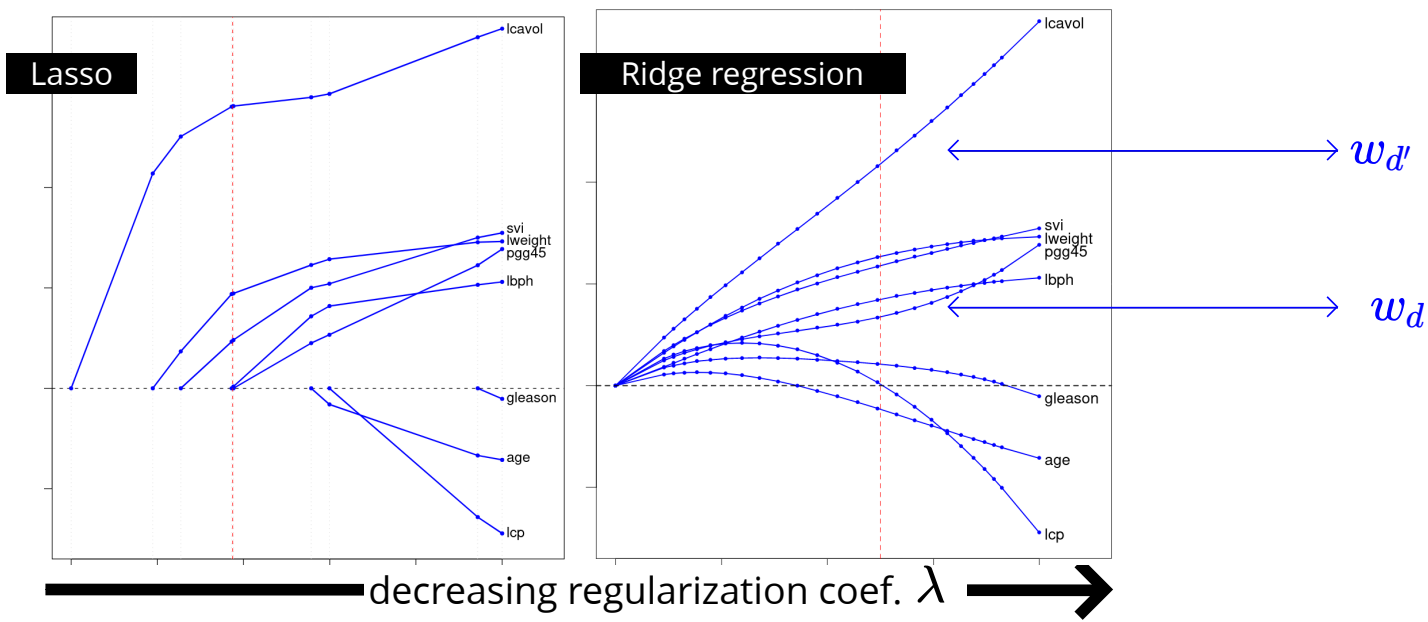
Lasso produces sparse weights (many are zero, rather than small)



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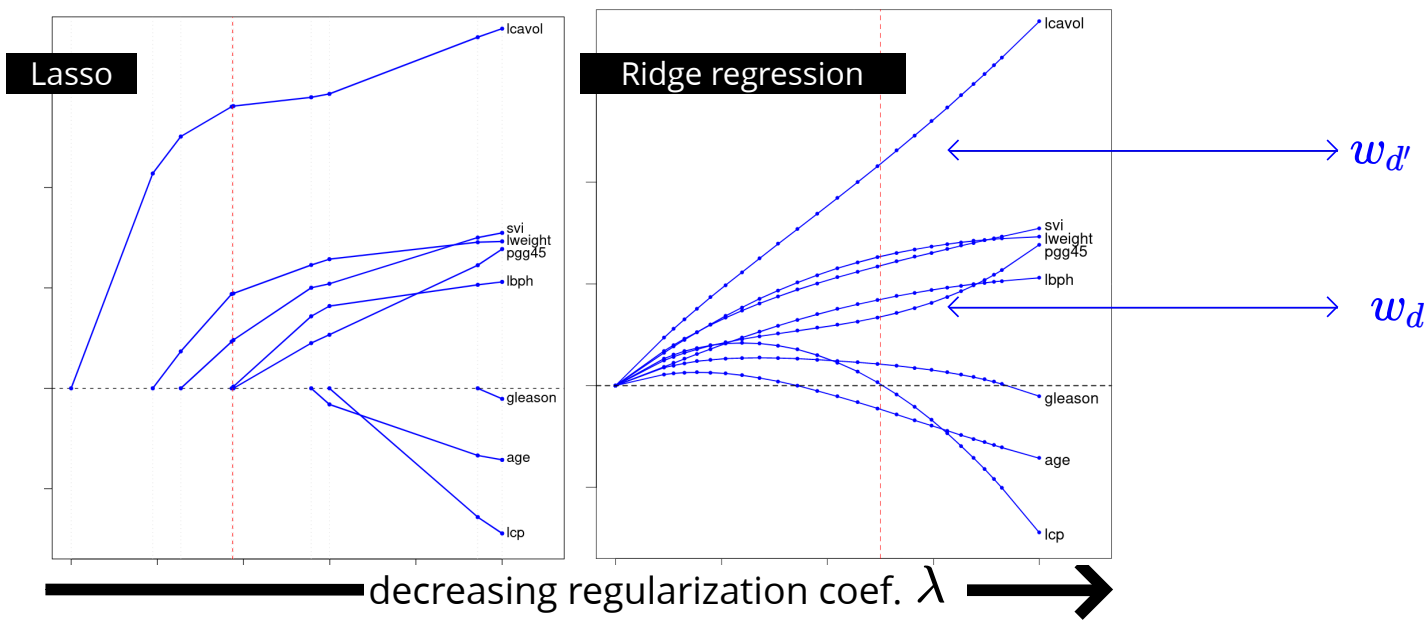
red-line is the optimal λ from cross-validation



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is equivalent to $\min_w J(w)$ *subject to* $||w||_p^p \leq \tilde{\lambda}$ for an appropriate choice of $\tilde{\lambda}$

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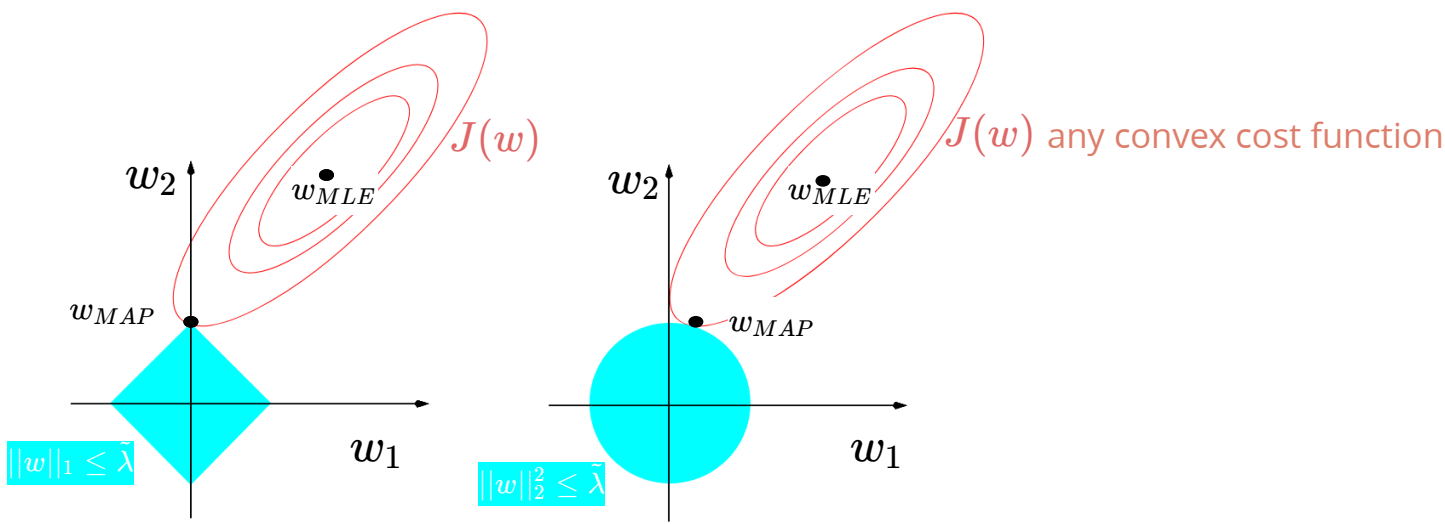

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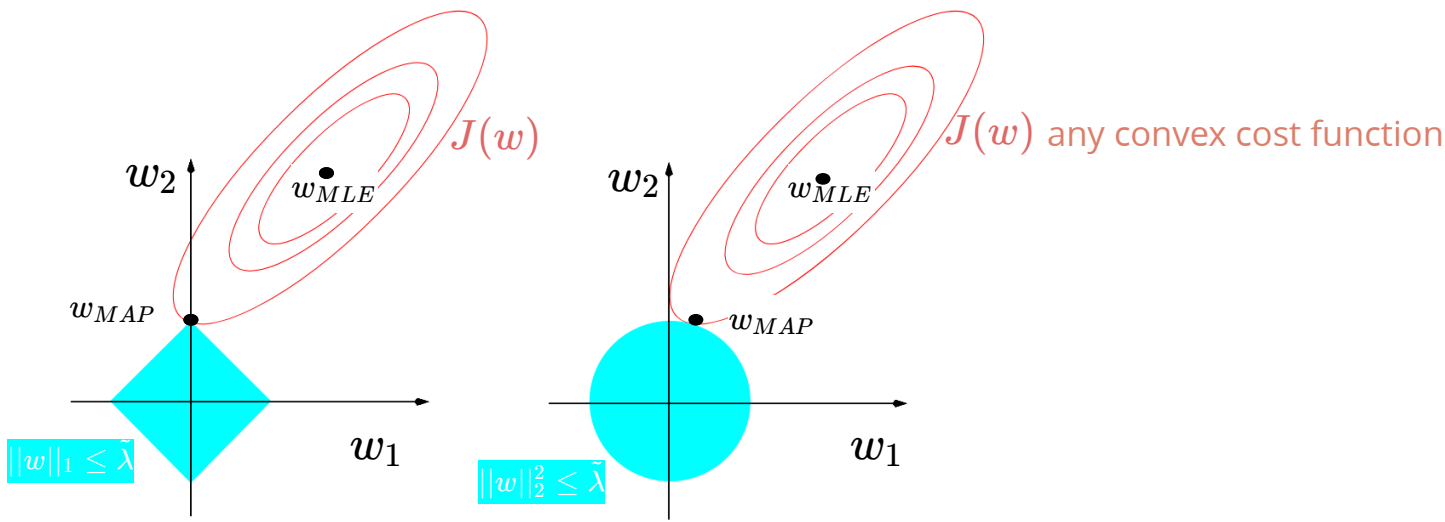
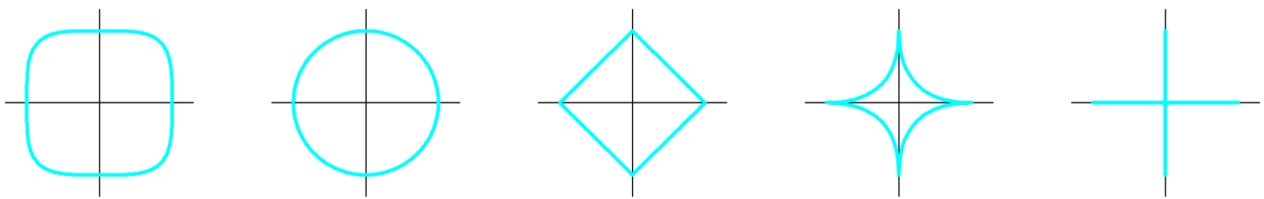
optimal solution with L1-regularization is more likely to have zero components



Subset selection



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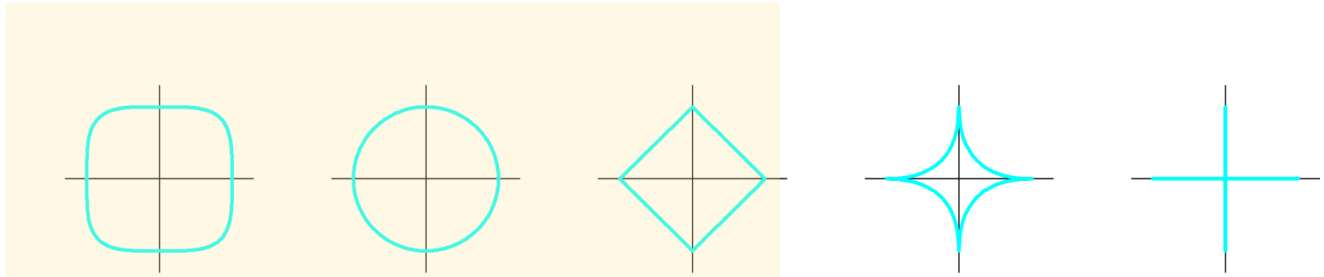
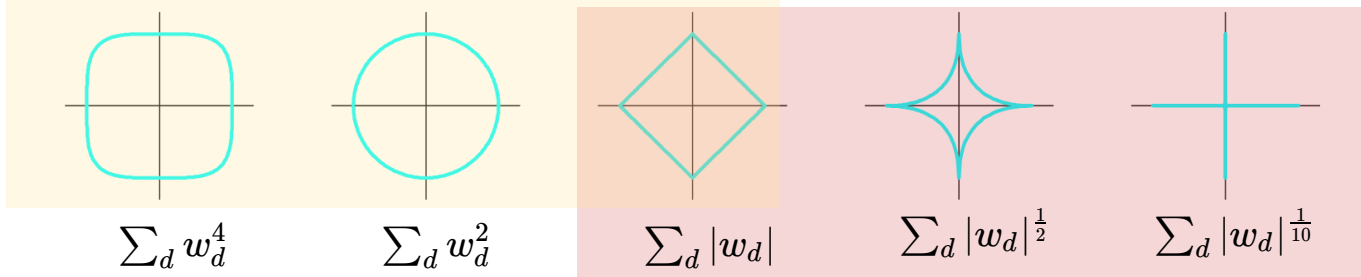


$\sum_d w_d^4$ $\sum_d w_d^2$ $\sum_d |w_d|$ $\sum_d |w_d|^{\frac{1}{2}}$ $\sum_d |w_d|^{\frac{1}{10}}$

Subset selection

p-norms with $p \geq 1$ are convex (easier to optimize)

p-norms with $p \leq 1$ induces sparsity



Subset selection

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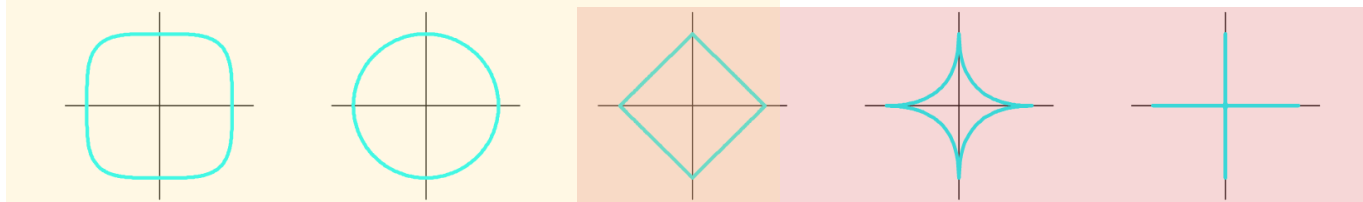

L_0 norm

closer to **0-norm**

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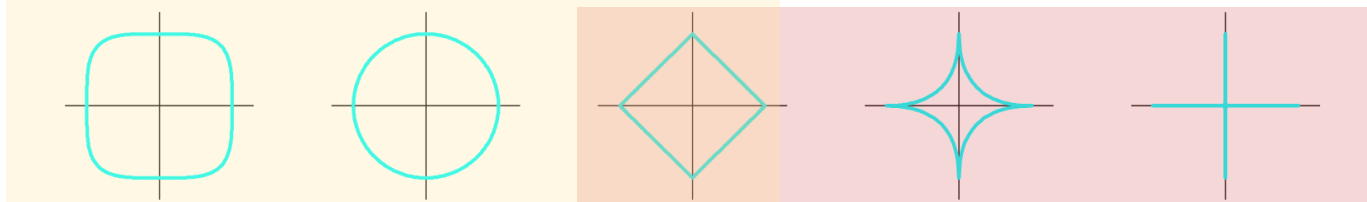

$\sum_d w_d^4$ $\sum_d w_d^2$ $\sum_d |w_d|$ $\sum_d |w_d|^{\frac{1}{2}}$ $\sum_d |w_d|^{\frac{1}{10}}$

L_0 norm — closer to **0-norm**

penalizes the **number of** non-zero features

$$J(w) + \lambda ||w||_0 = J(w) + \lambda \sum_d \mathbb{I}(w_d \neq 0)$$

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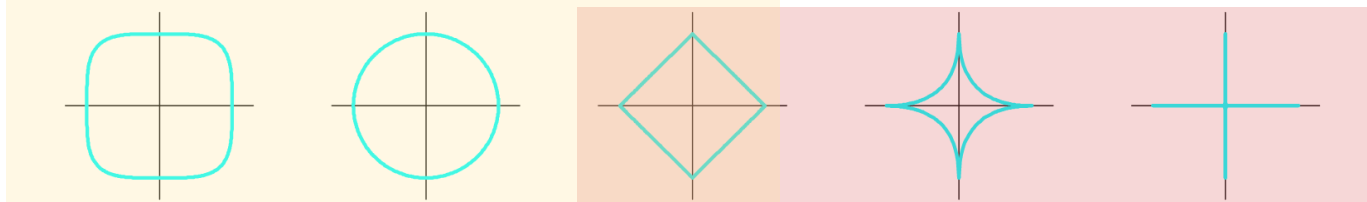

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a penalty of λ for each feature

performs feature selection

Subset selection

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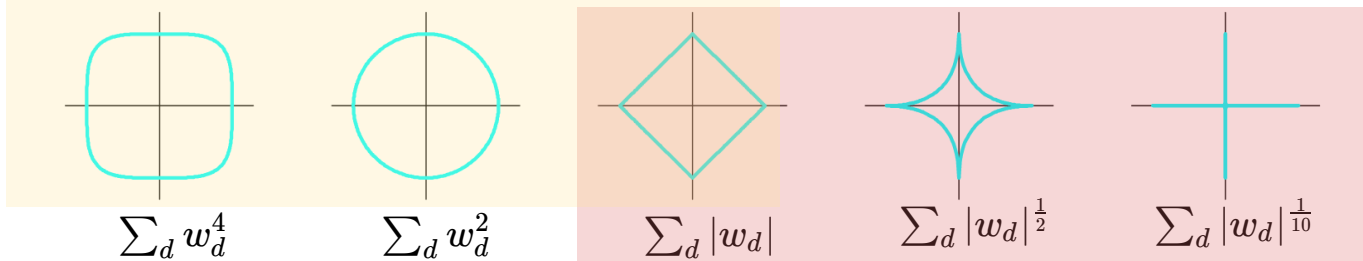

L_0 norm → closer to **0-norm**

optimizing this is a difficult *combinatorial problem*:

- search over all 2^D subsets

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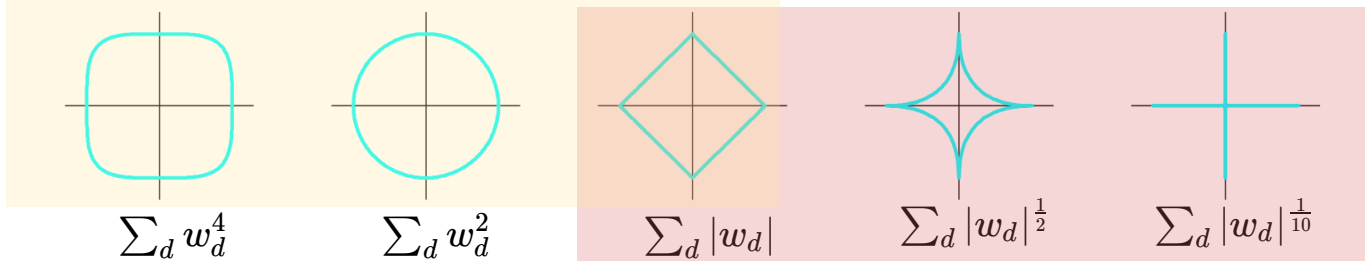

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L1 regularization is a viable alternative to L0 regularization

Bias-variance decomposition

for L2 loss

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for L2 loss

assume a true distribution $p(x, y)$

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what we care about is the expected loss (*aka risk*)

$$\mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - y)^2]$$

all blue items are random variables

Bias-variance decomposition

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Bias-variance decomposition

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what we care about is the expected loss (*aka risk*)

$$\mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - \underbrace{y}_{f(x)+\epsilon})^2]$$

Bias-variance decomposition

for L2 loss

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y: $f(x) + \epsilon$

$\hat{f}_{\mathcal{D}}(x)$: $\hat{f}_{\mathcal{D}}(x) + \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]$ add and subtract a term

Bias-variance decomposition

for L2 loss

what we care about is the expected loss (*aka risk*)

$$\mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - y)^2] = \mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - y + \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2]$$

$f(x) + \epsilon$

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the remaining terms evaluate to zero (check for yourself!)

$$= \mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2] + \mathbb{E}[(f(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2] + \mathbb{E}[\epsilon^2]$$

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variance | bias | unavoidable noise error

Bias-variance decomposition

for L2 loss

the expected loss is decomposed to:

image: P. Domingos' posted article

Bias-variance decomposition

for L2 loss

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bias: how average over all datasets differs from the regression function

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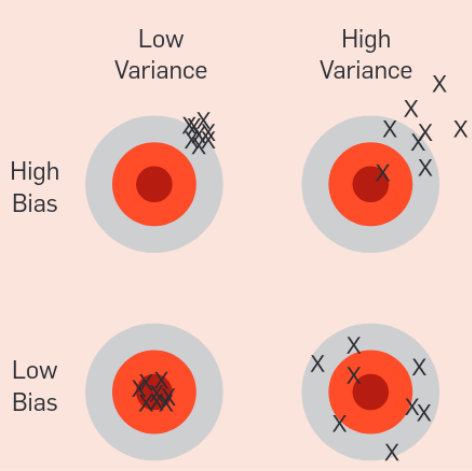

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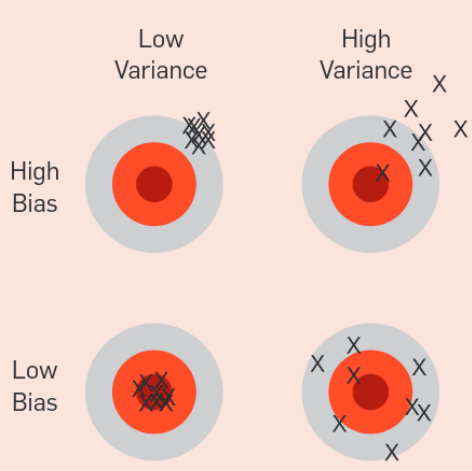
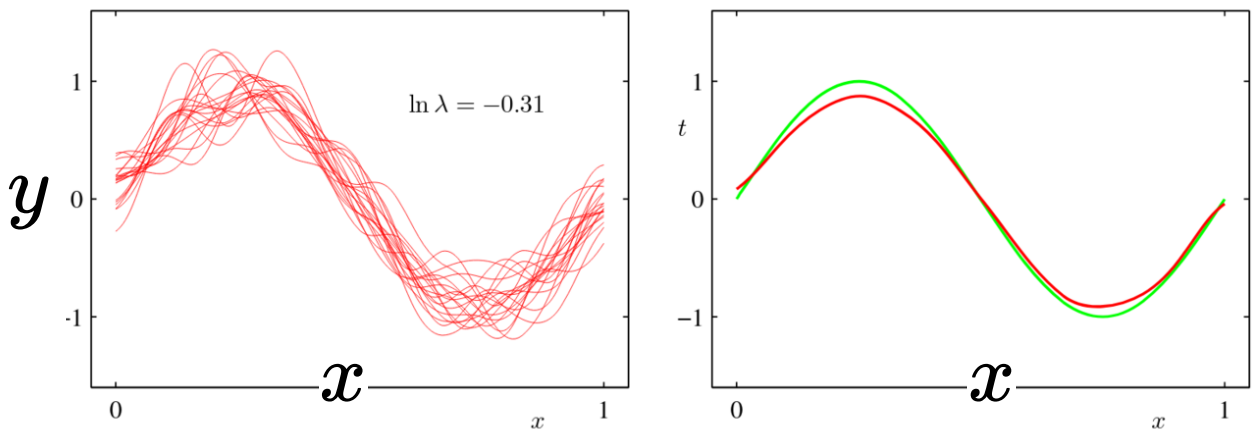


different models vary in their trade off between error due to bias and variance

- simple models: often more biased
- complex models: often have more variance

image: P. Domingos' posted article

Example: bias vs. variance

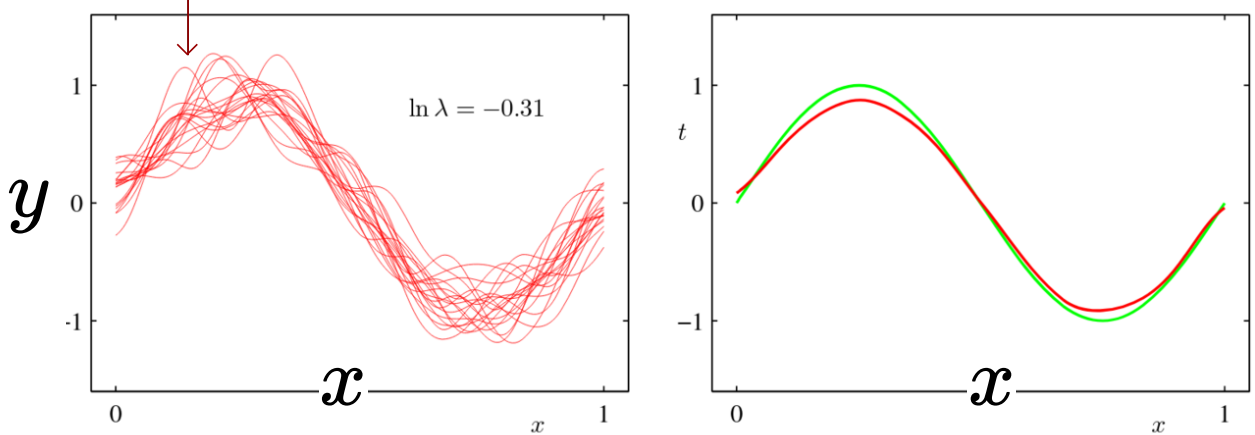


Example: bias vs. variance

models for different datasets $\hat{f}_{\mathcal{D}}$

using Gaussian bases

random datasets of size N=25 instances are not shown



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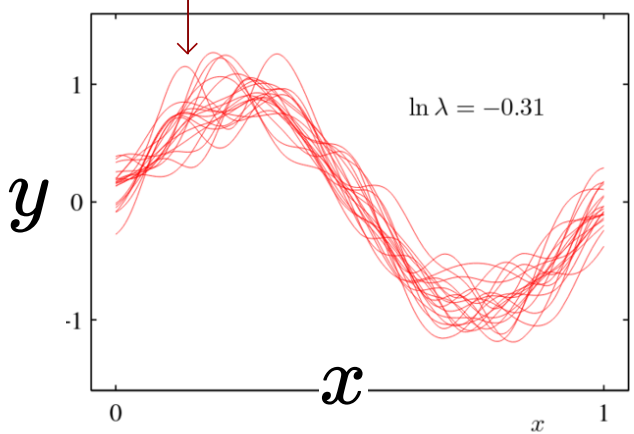
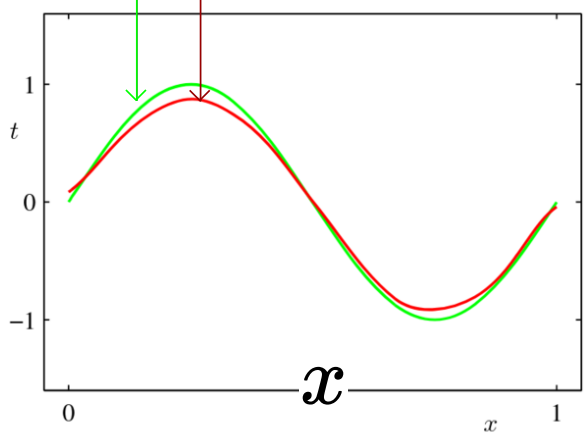


true model f

their average $\mathbb{E}[\hat{f}_{\mathcal{D}}]$



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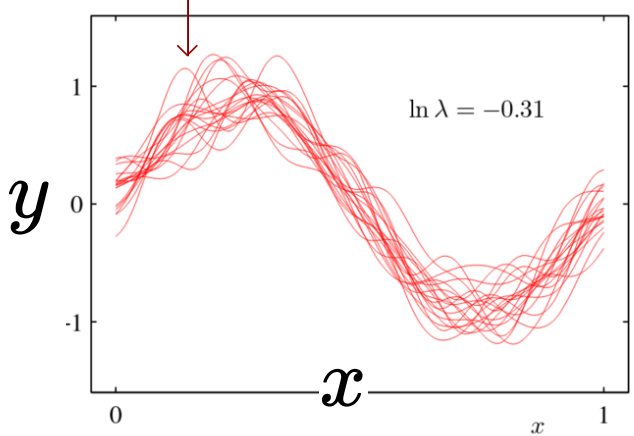
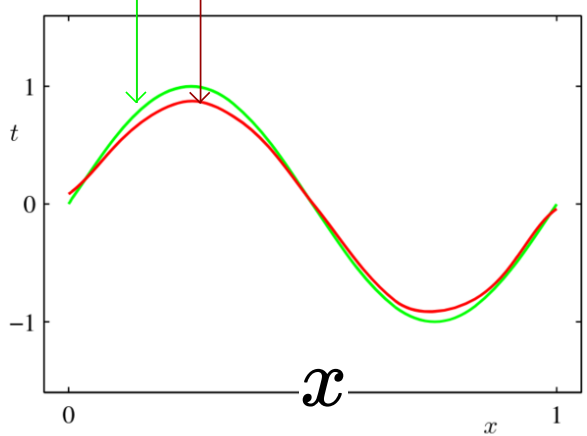


variance is the average difference (in squared L2 norm) between these curves and their average

true model f

their average $\mathbb{E}[\hat{f}_{\mathcal{D}}]$



bias is the difference (in L2 norm) between two curves

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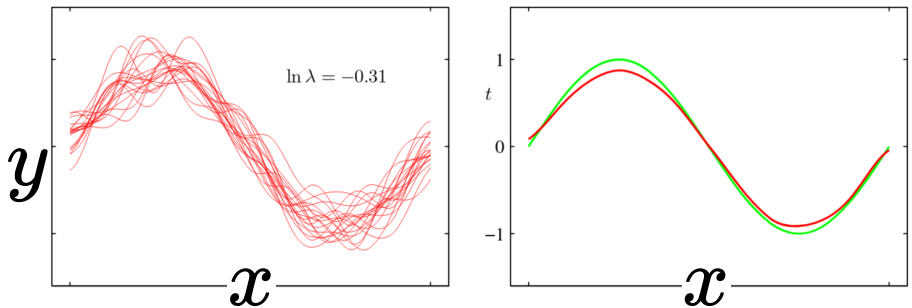

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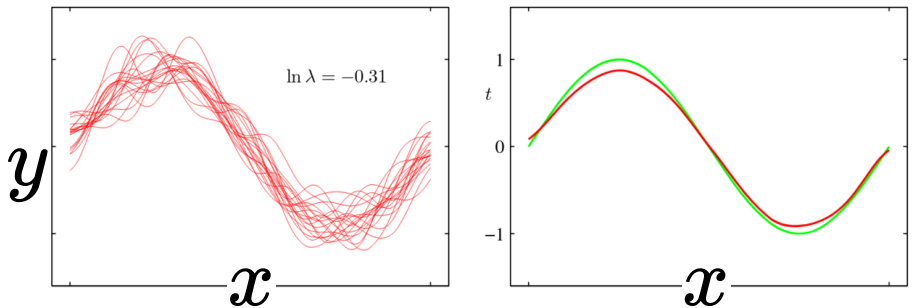
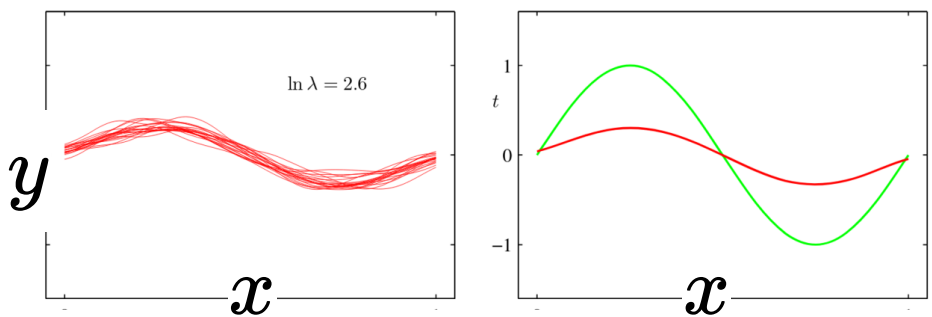


using larger regularization penalty: higher bias - lower variance



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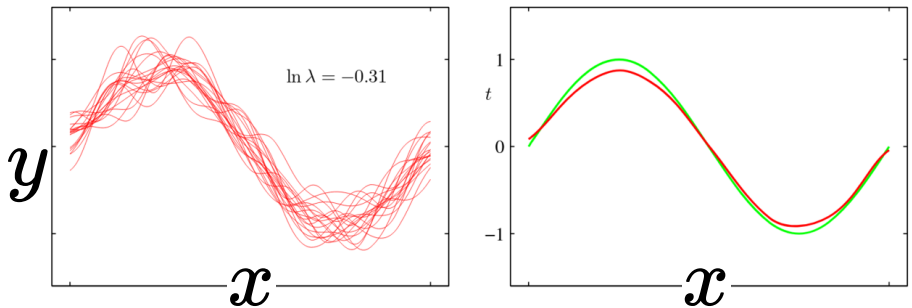
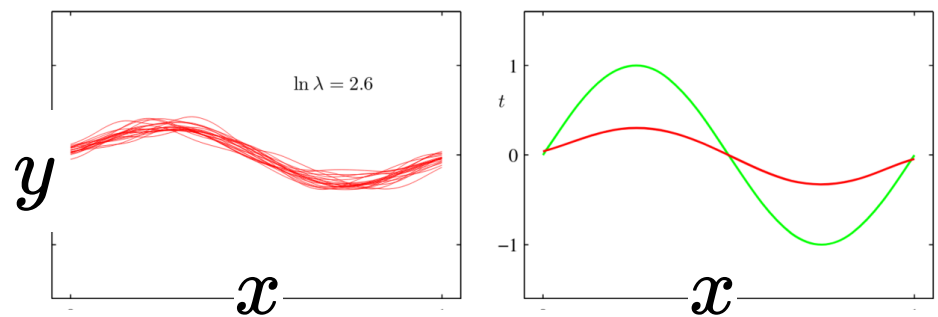


side note

the average fit is very good, despite high variance

model averaging: uses "average" prediction of expressive models to prevent overfitting

using larger regularization penalty: higher bias - lower variance



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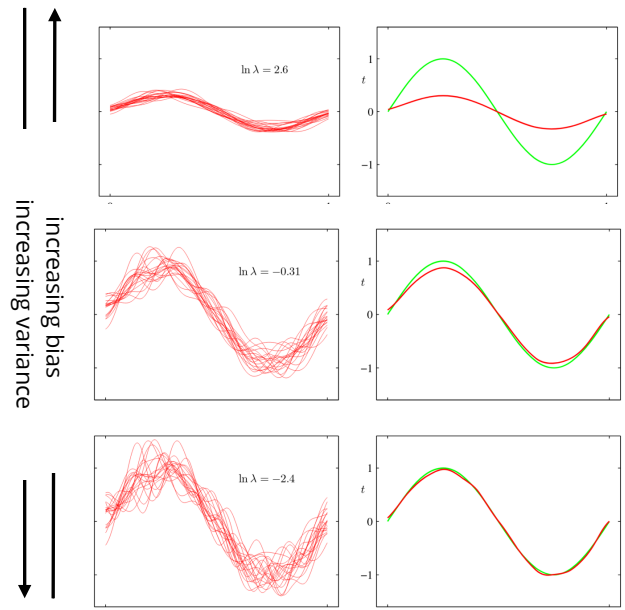
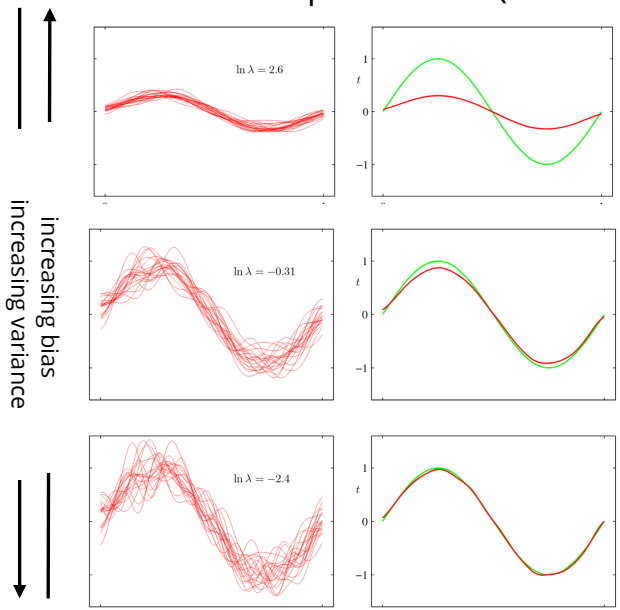
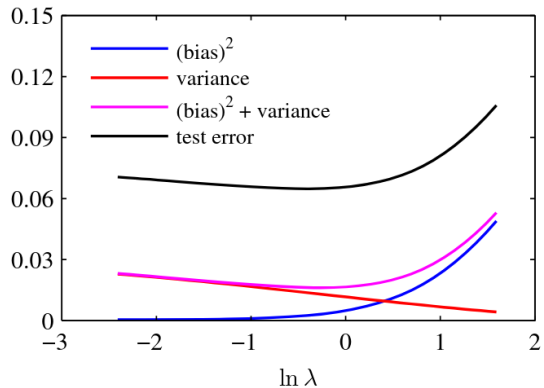


Example: bias vs. variance

the lowest expected loss (test error) is somewhere between the two extremes





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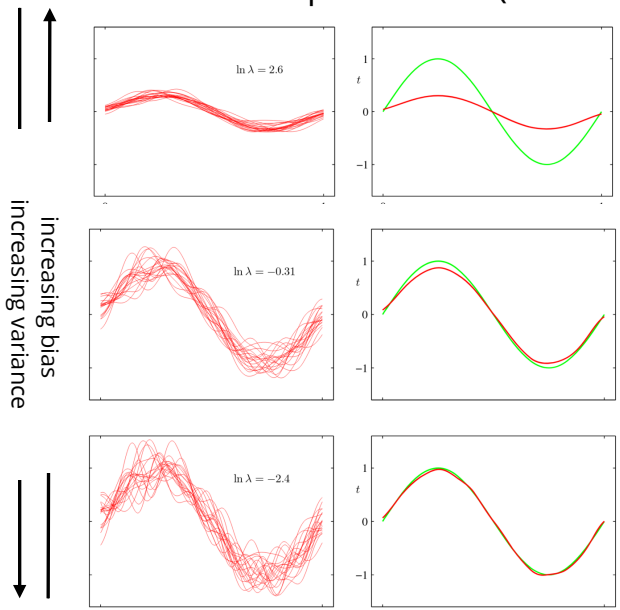
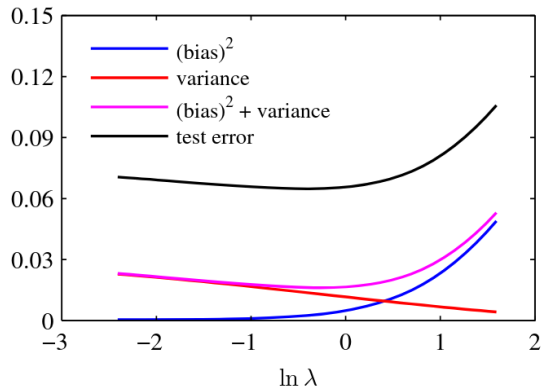
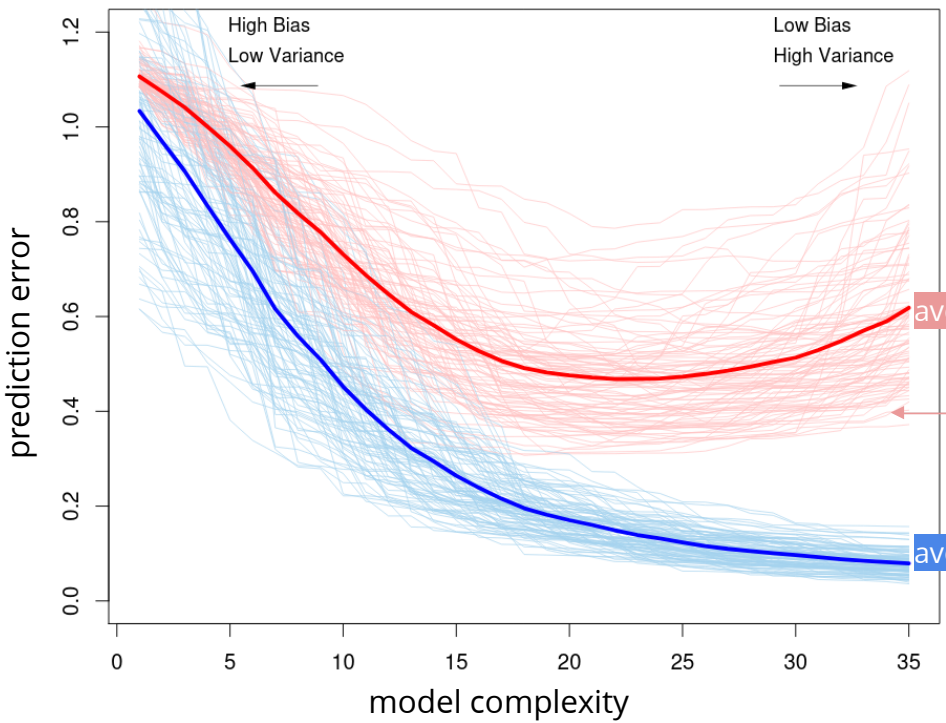




in reality, we don't have access to the true model

how to decide which model to use?

Big picture!



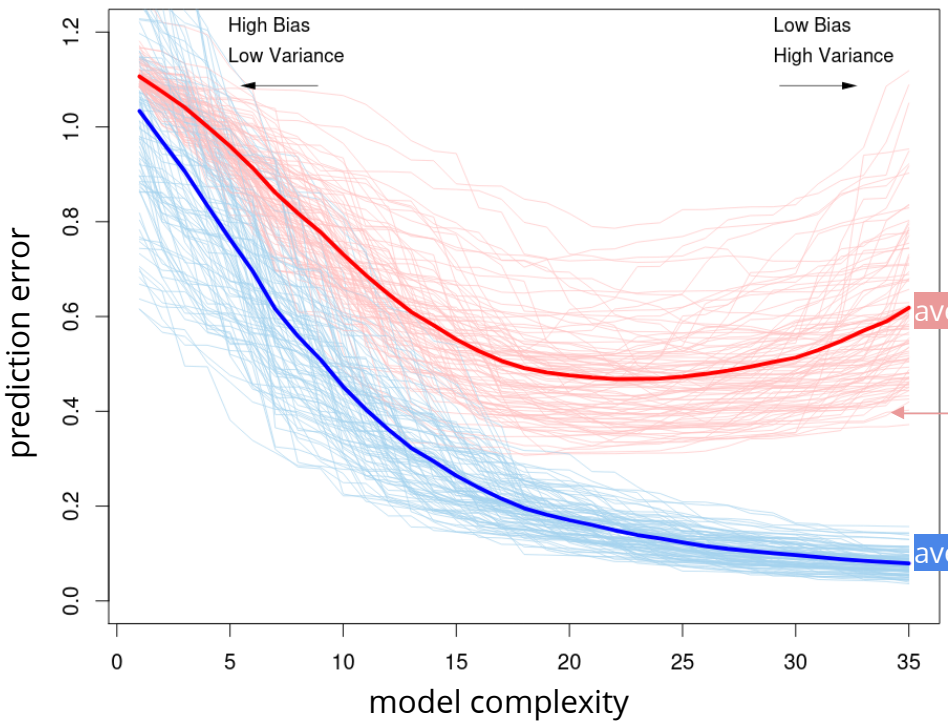
average test error

error for random dataset $\mathcal{D}$

average training error

Big picture!

high variance in more complex models means that test and training error can be very different



average test error

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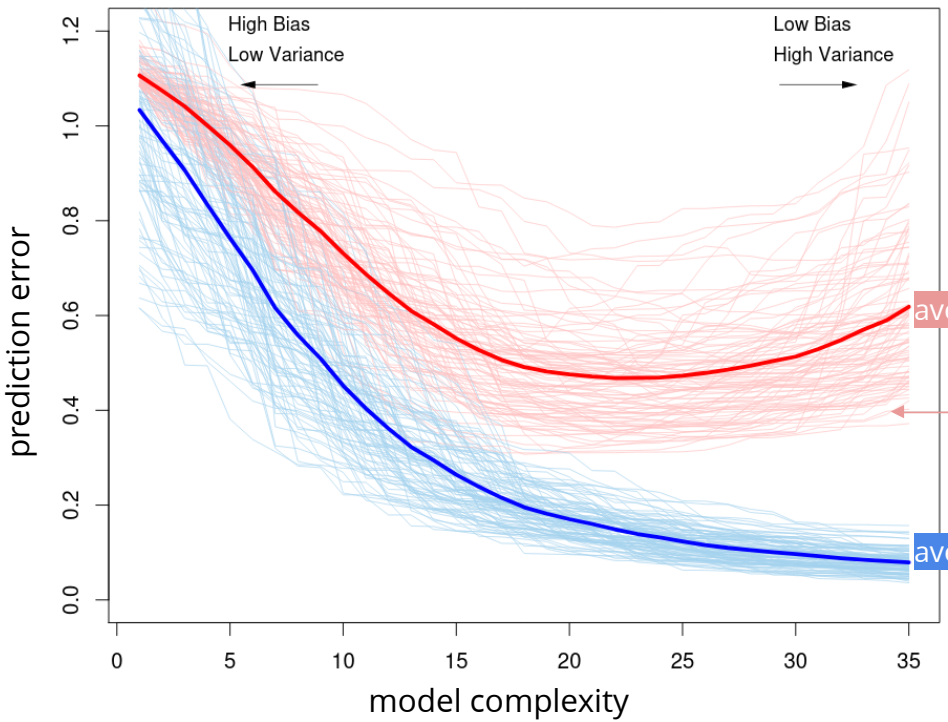
Big picture!

high variance in more complex models means that test and training error can be very different
high bias in simplistic models means that training error can be high



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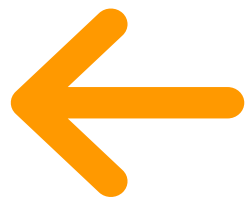
Model selection

how to pick the model with lowest expected loss / test error?

use a **validation set** (and a separate test set for final assessment)



regularization bound the test error by bounding

- training error
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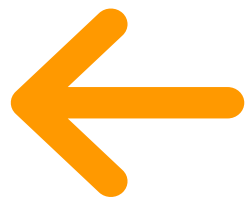

regularization bound the test error by bounding

- training error
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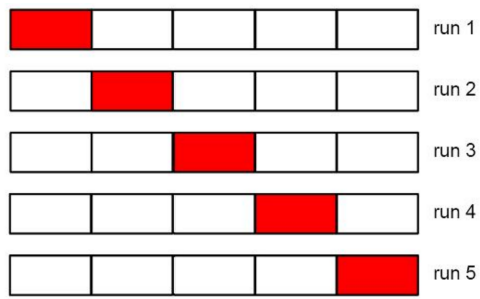
in the end we may have to use a validation set to find the right amount of regularization

Cross validation

getting a more reliable estimate of test error using validation set

K-fold cross validation(CV)

- randomly partition the data into K *folds*
- use K-1 for training, and 1 for validation
- report average/std of the validation error over all folds



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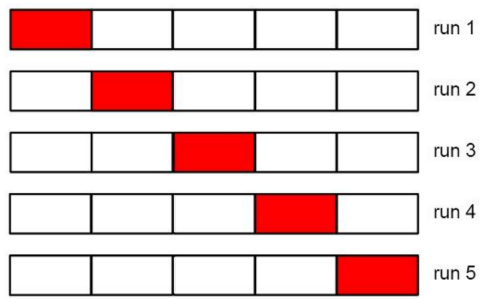

leave-one-out CV: extreme case of k=N

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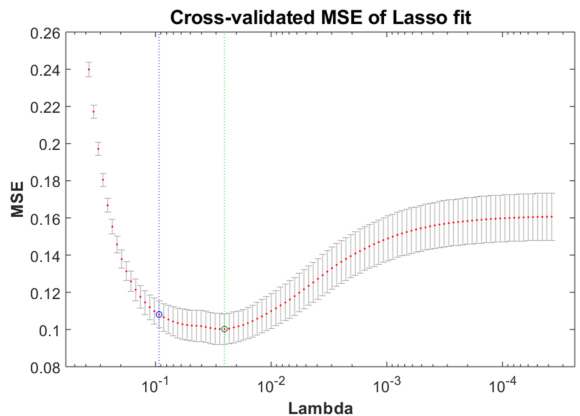

image credit: Thanh Nguyen et al'19

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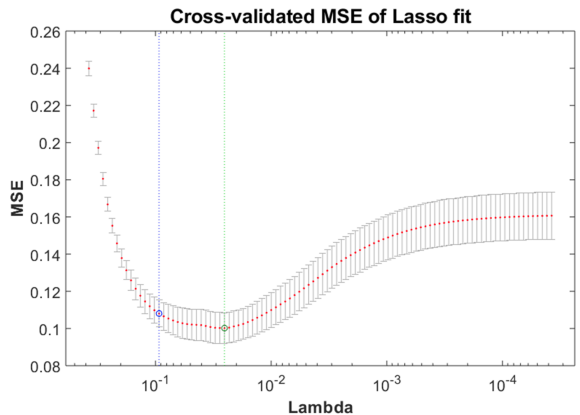

once the hyper-parameters are selected, we can use the whole set for training

use test set for the **final** assessment

image credit: Thanh Nguyen et al'19

Evaluation

evaluation metric can be different from the optimization objective

confusion matrix is a CxC table that compares truth-vs-prediction

for **binary classification**:

	Truth		Σ
Result	TP	FP	RP
	FN	TN	RN
Σ	P	N	

Evaluation

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confusion matrix is a CxC table that compares truth-vs-prediction

for **binary classification**:

	Truth		Σ
Result	TP	FP	RP
	FN	TN	RN
Σ	P	N	

some **evaluation metrics**
(based on the confusion table)

$$Accuracy = \frac{TP+TN}{P+N}$$

$$Error\ rate = \frac{FP+FN}{P+N}$$

$$Precision = \frac{TP}{RP}$$

$$Recall = \frac{TP}{P}$$

$$F_1 score = 2\frac{Precision \times Recall}{Precision + Recall}$$

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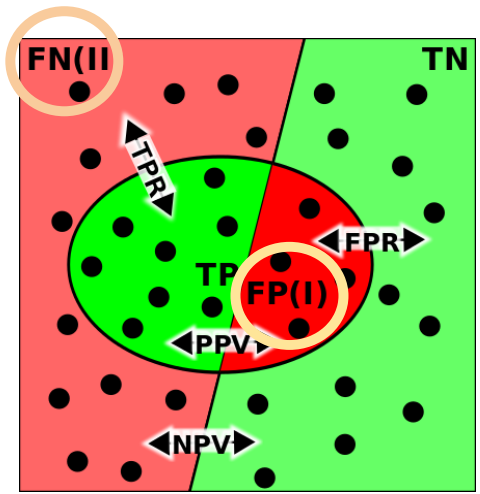
type I vs type II error



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if we produce class score (probability)
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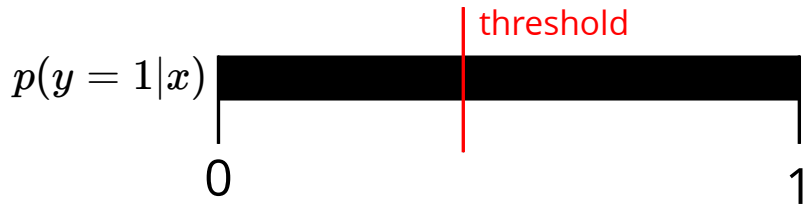

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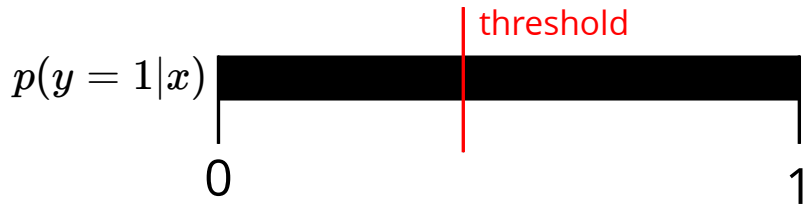

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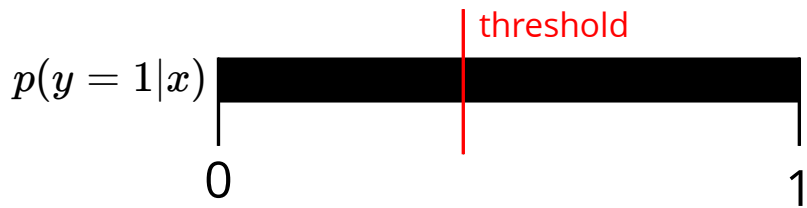

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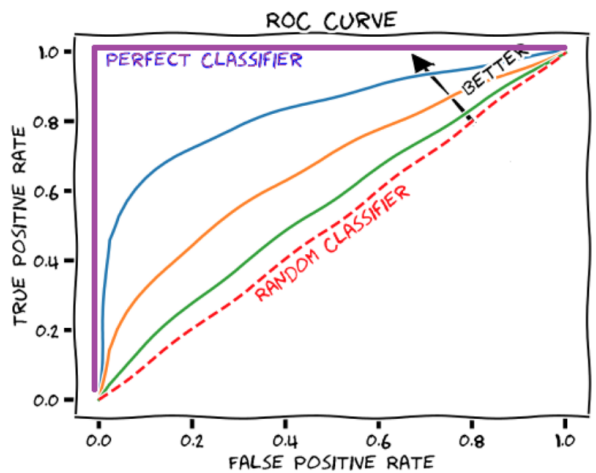
Receiver Operating Characteristic **ROC curve**

TPR = TP/P (**recall**, sensitivity)
FPR = FP/N (**fallout**, false alarm)



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- regularization bounds this gap by penalizing model complexity
  - L1 & L2 regularization
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- (cross) validation for model selection