Applied Machine Learning

Regularization

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Learning objectives

- intuition for model complexity and overfitting
- regularization penalty (L1 & L2)
- probabilistic interpretation

recall

Linear regression

model: $\hat{y} = f_w(x) = w^\top x \ : \mathbb{R}^D \to \mathbb{R}$

cost function: $J_w = \frac{1}{N} \sum_n \frac{1}{2}(y^{(n)} - \hat{y}^{(n)})^2 = \frac{1}{2}||y - Xw||^2$

how to find w^*? closed form solution: $w^* = (X^\top X)^{-1} X^\top y$

Or use gradient descent

partial derivatives: $\frac{\partial}{\partial w_d} J_w = \frac{1}{N} \sum_n (\hat{y}^{(n)} - y^{(n)}) x_d^{(n)}$

gradient (all partial derivatives): $\nabla J(w) = \frac{1}{N} \sum_n (\hat{y}^{(n)} - y^{(n)}) x^{(n)} = \frac{1}{N} X^\top (\hat{y} - y)$

optimization with gradient descent: repeat until stopping criterion: $w^{\{t+1\}} \leftarrow w^{\{t\}} - \alpha \nabla J(w^{\{t\}})$

what if **linear fit is not the best**?
how to increase the model's expressiveness?
$\Rightarrow$ use nonlinear basis to create new nonlinear features from the existing ones

recall

Nonlinear basis functions

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

with nonlinear bases $f_w(x) = \sum_d w_d \phi_d(x)$

linear least squares solution $(\Phi^\top \Phi) w^* = \Phi^\top y$

replacing X with Φ

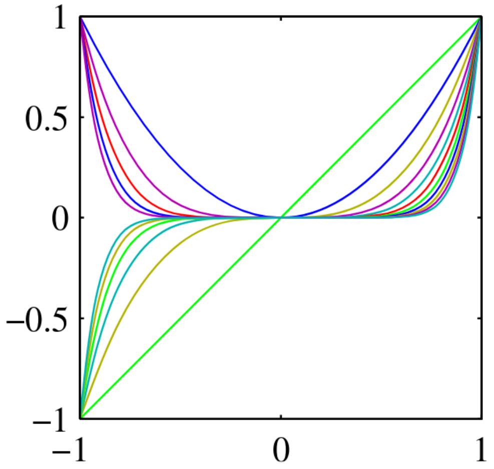
a (nonlinear) feature

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

one instance

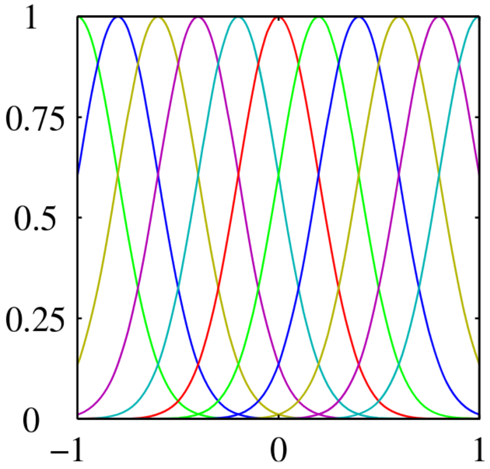
Nonlinear basis functions

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



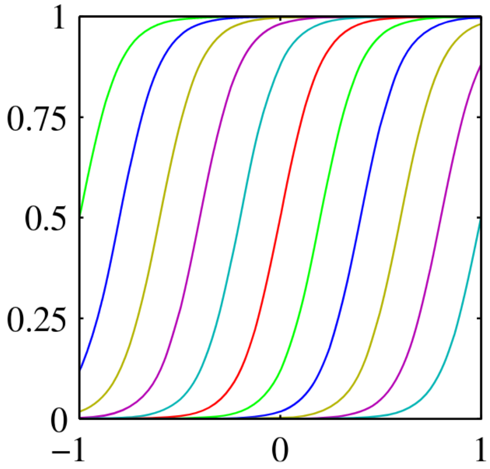
polynomial bases

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



Gaussian bases

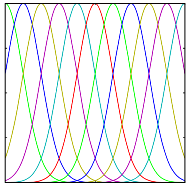
$$\phi_k(x) = e^{-\frac{(x-\mu_k)^2}{s^2}}$$



Sigmoid bases

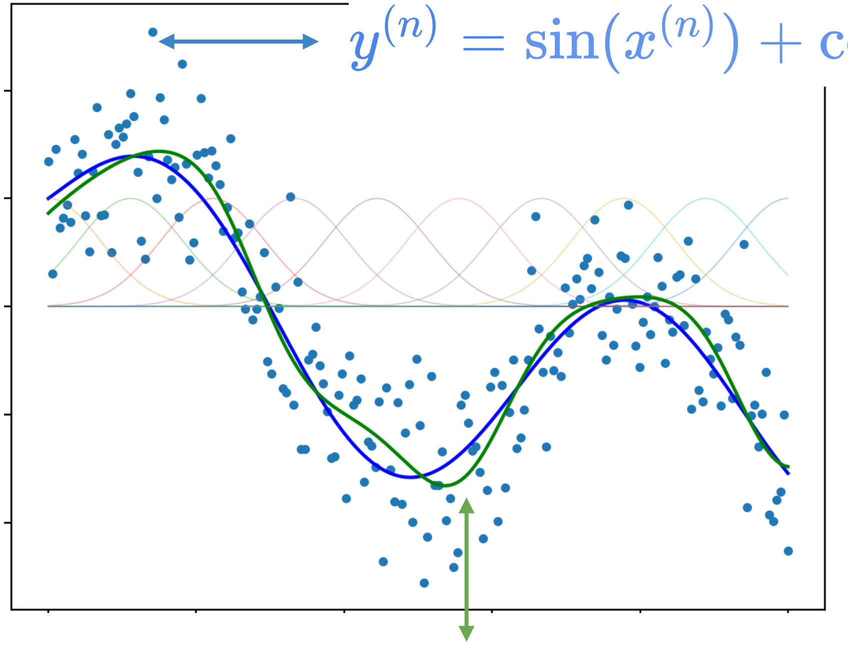
$$\phi_k(x) = \frac{1}{1+e^{-\frac{x-\mu_k}{s}}}$$

Example: Gaussian bases



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

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



our fit to data using 10 Gaussian bases

prediction for a new instance

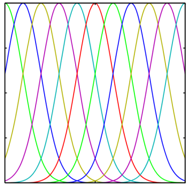
$$f(x') = \phi(x')^\top (\Phi^\top \Phi)^{-1} \Phi^\top y$$

new instance

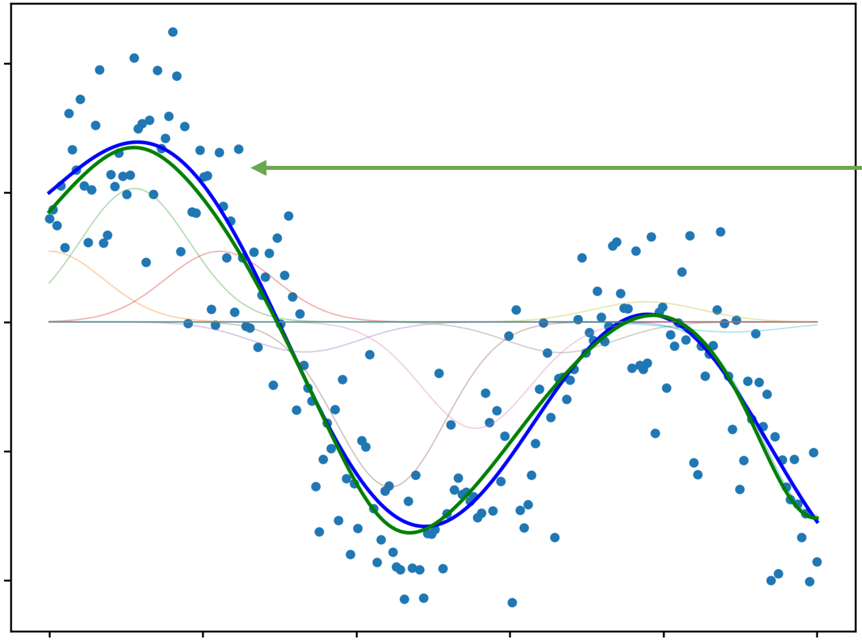
features evaluated for the new point

w found using LLS

Example: Gaussian bases



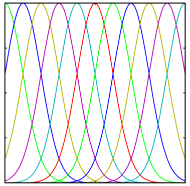
$$\phi_k(x) = e^{-\frac{(x-\mu_k)^2}{s^2}}$$



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

why not more?

Example: Gaussian bases



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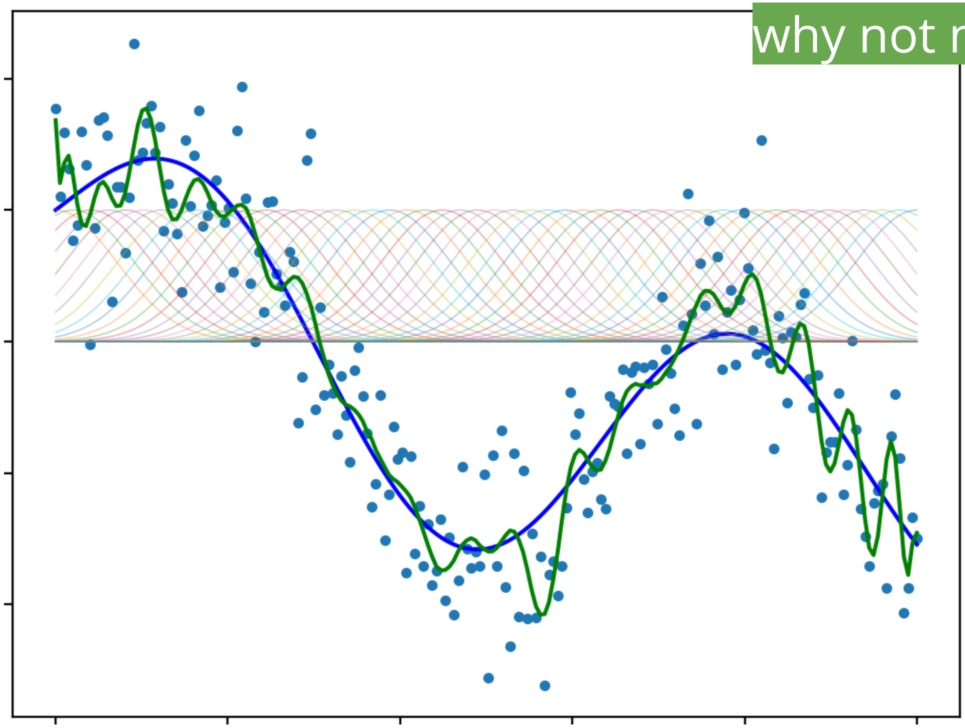
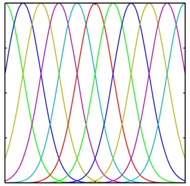


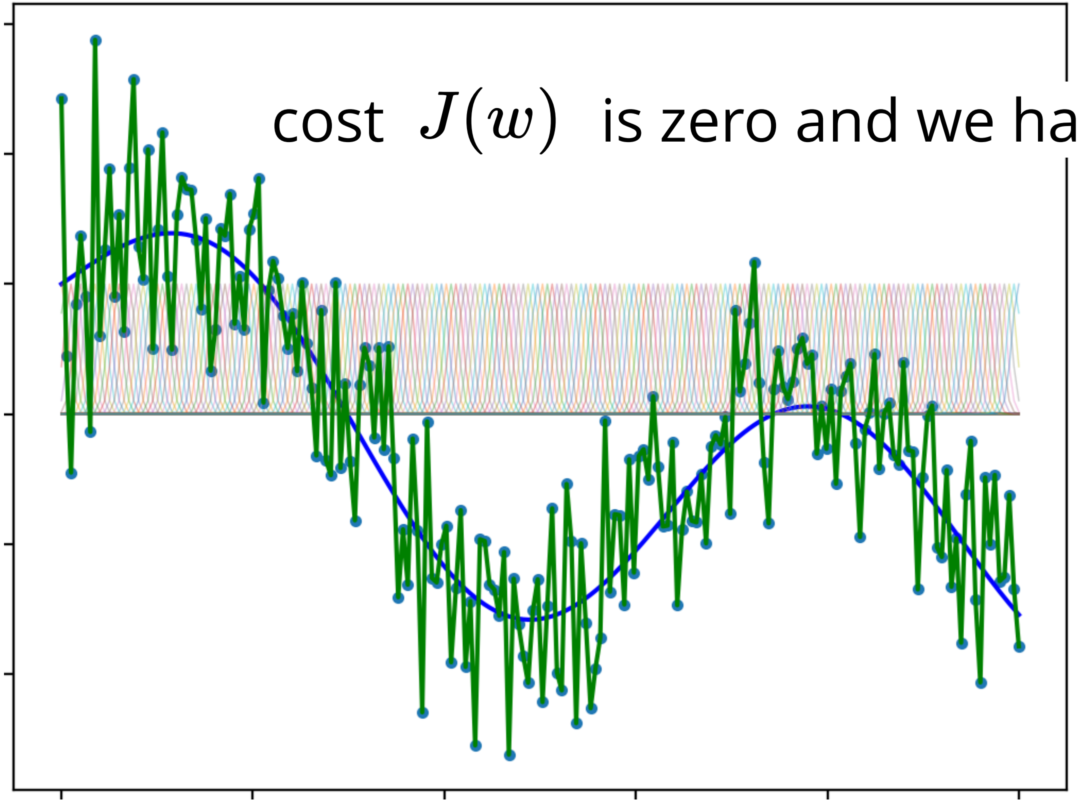
why not more?

using 50 bases!

Example: Gaussian bases



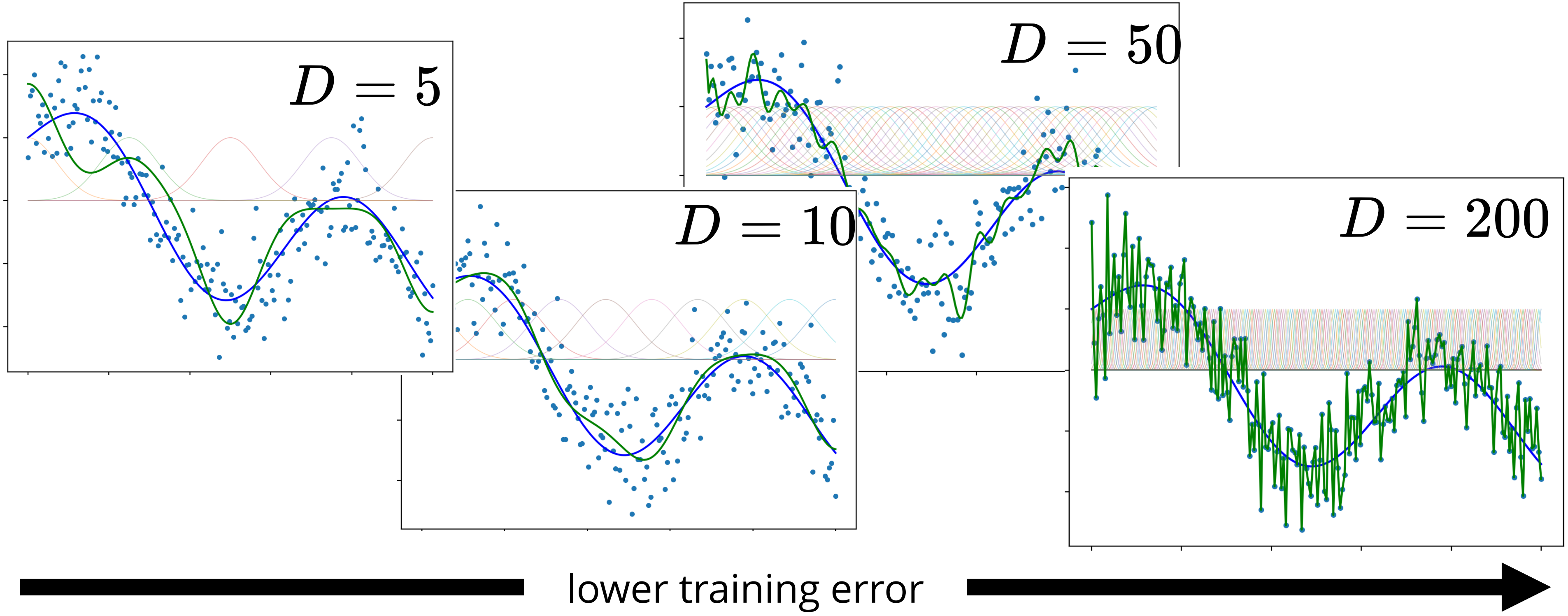
$$\phi_k(x) = e^{-\frac{(x-\mu_k)^2}{s^2}}$$



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

using 200, thinner bases (s=.1)

Generalization?

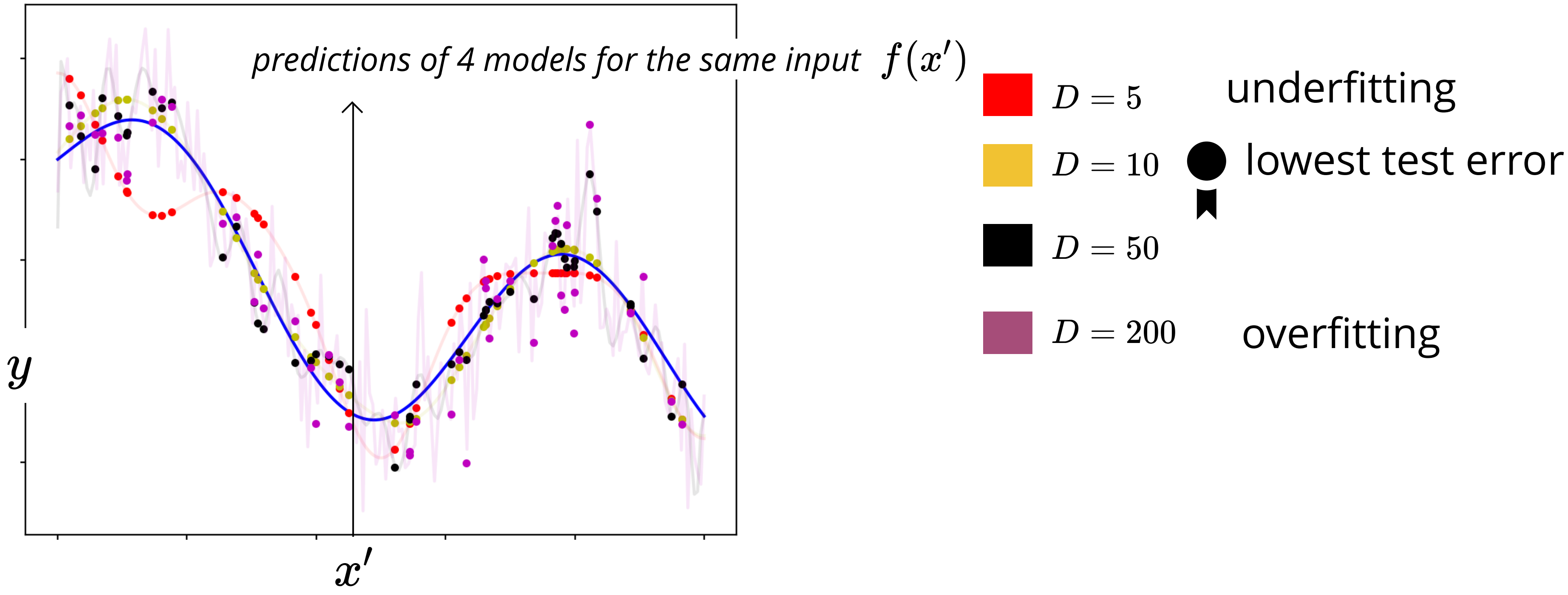


lower training error

which one of these models performs better at test time?

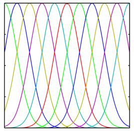
Overfitting

which one of these models performs better at test time?



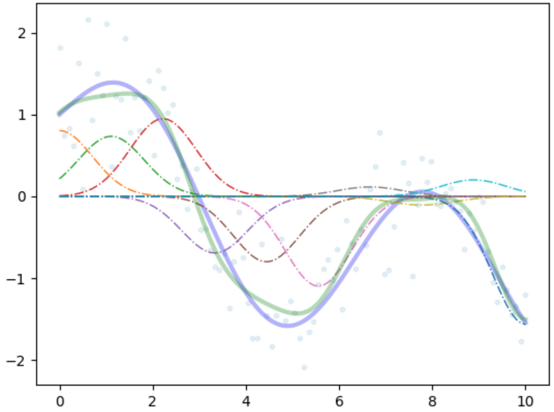
An observation

when overfitting, we sometimes see large weights

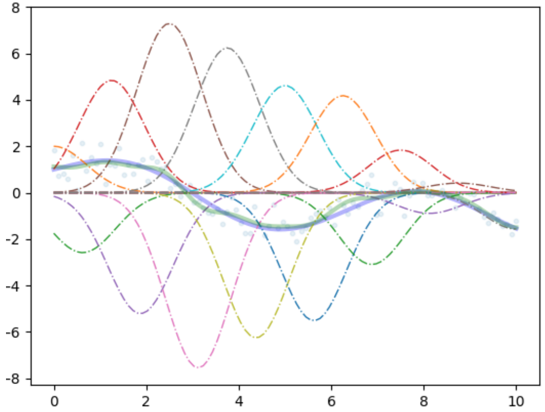


dashed lines are $w_d \phi_d(x) \quad \forall d$ $\qquad f_w(x) = \sum_d w_d \, \phi_d(x)$

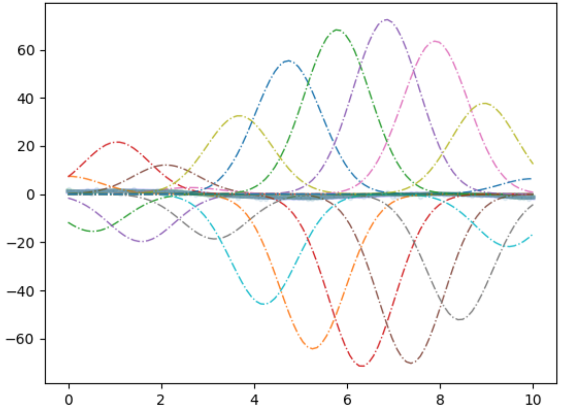
$D = 10$



$D = 17$



$D = 20$



idea: penalize large parameter values

Ridge regression

also known as

L2 regularized linear least squares regression:

$$J(w) = \frac{1}{2}||Xw - y||_2^2 + \frac{\lambda}{2}||w||_2^2$$

sum of squared error

$$\frac{1}{2}\sum_n (y^{(n)} - w^\top x)^2$$

squared L2 norm of w

$$w^T w = \sum_d w_d^2$$

regularization parameter $\lambda > 0$ controls the strength of regularization

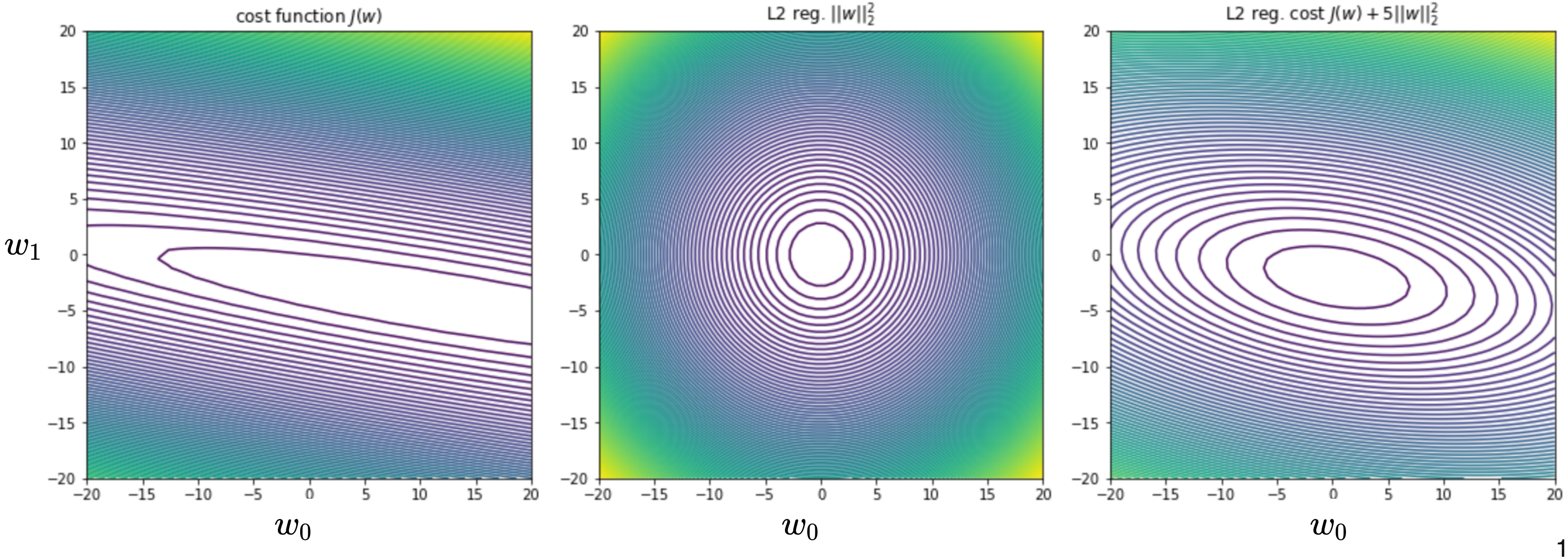
a good practice is to **not** penalize the intercept $\lambda(||w||_2^2 - w_0^2)$

λ is a hyper-parameter (use a validation set or cross-validation to pick the best value)

Ridge regression example

Visualizing the effect of regularization on the cost function

is the new cost function convex? $\frac{1}{2N}\sum_{x,y\in\mathcal{D}}(y - w^\top x)^2 + \frac{\lambda}{2}||w||_2^2$



Ridge regression

set the derivative to zero $J(w) = \frac{1}{2}\sum_{x,y\in\mathcal{D}}(y - w^\top x)^2 + \frac{\lambda}{2}w^\top w$

$$\nabla J(w) = \sum_{x,y\in\mathcal{D}} x(w^\top x - y) + \lambda w$$

$$= X^\top(Xw - y) + \lambda w = 0$$

when using gradient descent, this term reduces the weights at each step **(weight decay)**

linear system of equations $(X^\top X + \lambda \mathbf{I})w = X^\top y$

$$w = (X^\top X + \lambda \mathbf{I})^{-1} X^\top y$$

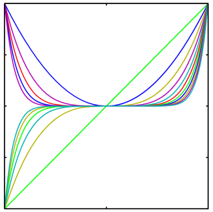
the only part different due to regularization

λI makes it invertible, adds a small value to the diagonals $X^\top X$

we can have linearly dependent features

the solution will be unique!

Example: polynomial bases

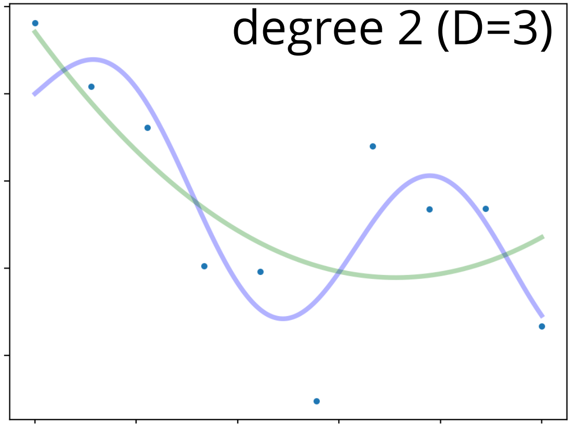


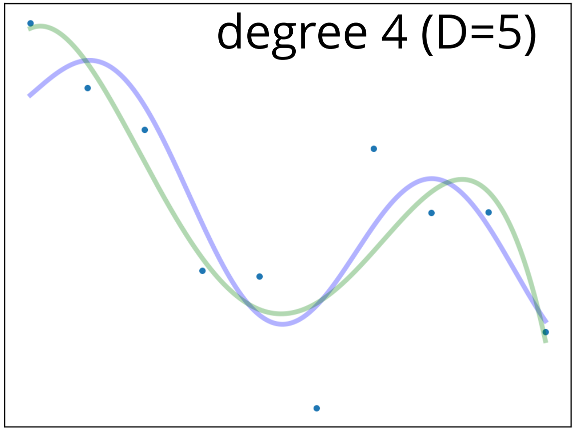
polynomial bases

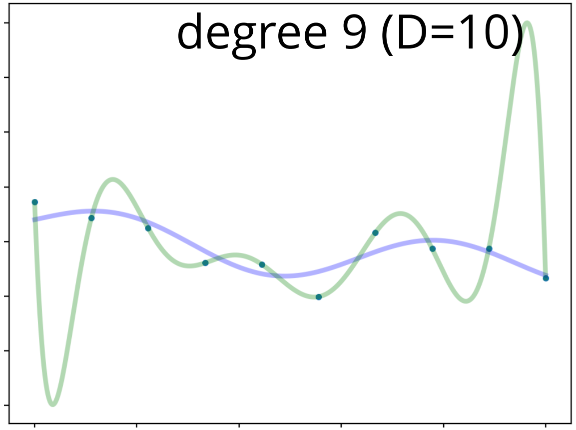
$$\phi_k(x) = x^k$$

Without regularization:

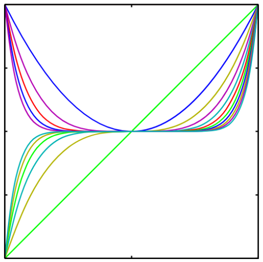
- using D=10 we can perfectly fit the data (high test error)







Example: polynomial bases

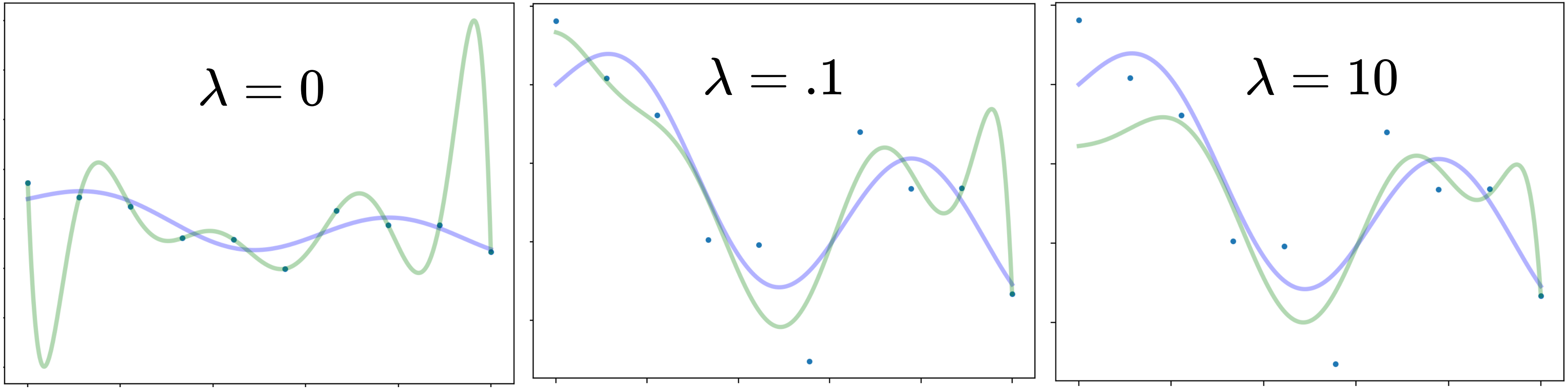


polynomial bases

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

with regularization:

- fixed D=10, changing the amount of regularization



Probabilistic interpretation

recall linear regression & logistic regression maximize log-likelihood

$$w^{MLE} = \arg\max_w p(y|X, w)$$

linear regression $$w^{MLE} = \arg\max_w \prod_{x,y \in \mathcal{D}} \mathcal{N}(y|w^\top x, \sigma^2)$$

logistic regression $$w^{MLE} = \arg\max_w \prod_{x,y \in \mathcal{D}} \text{Bernoulli}(y; \sigma(w^\top x))$$

can we do Bayesian inference instead of maximum likelihood?

$$p(w|y, X) \propto p(w)p(y|w, X)$$

posterior prior likelihood

Maximum a Posteriori (MAP)

can we do Bayesian inference instead of maximum likelihood?

$$p(w|y, X) \propto p(w)p(y|w, X)$$

posterior prior likelihood

in general, this is expensive, but there's a cheap compromise:

MAP estimate $$w^{MAP} = \arg\max_w p(w)p(y|X, w)$$

$$= \arg\max_w \log p(y|X, w) + \log p(w)$$

likelihood: original objective prior

all that is changing is the additional penalty on w

Gaussian Prior

MAP estimate $w^{MAP} = \arg\max_w \log p(y|X, w) + \log p(w)$

prior

assume independent zero-mean Gaussians

$\mathcal{N}(\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$

$$\log p(w) = \log \prod_{d=1}^{D} \mathcal{N}(w_d | 0, \tau^2) = -\sum_d \frac{w^2}{2\tau^2} + \text{const.}$$

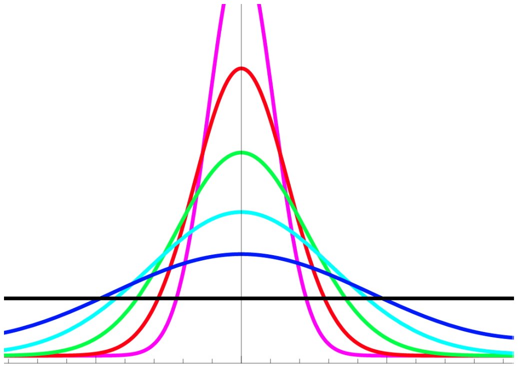
does not depend on w

so it doesn't affect the optimization

lets call $\frac{1}{\tau^2} \to \lambda$

then we get the L2 regularization penalty $\frac{\lambda}{2}||w||_2^2$

smaller variance of the prior τ gives larger regularization λ



Laplace prior

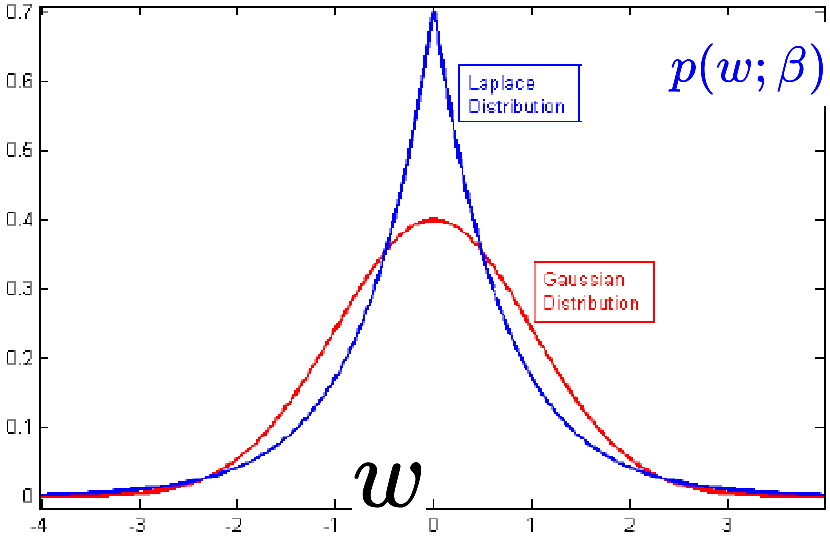
another notable choice of prior is the Laplace distribution

minimizing negative log-likelihood $\rightarrow$ $\sum_d \log p(w_d) = -\sum_d \frac{1}{\beta}|w_d| = -\frac{1}{\beta}||w||_1$

L1 norm of w

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

(least absolute shrinkage and selection operator)



$p(w;\beta) = \frac{1}{2\beta}e^{-\frac{|w|}{\beta}}$ notice the peak around zero

image from here

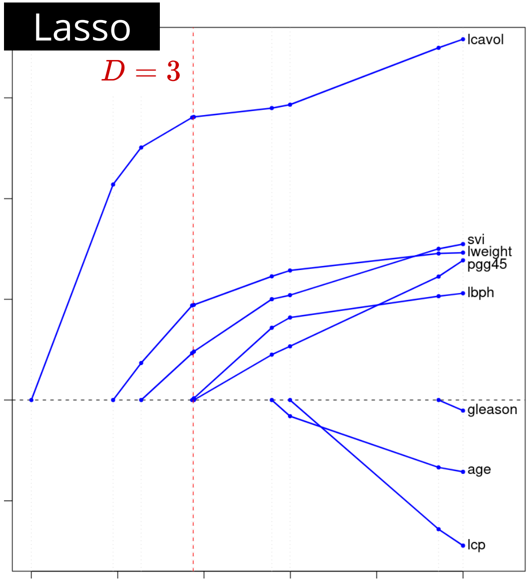
L_1 vs L_2 regularization

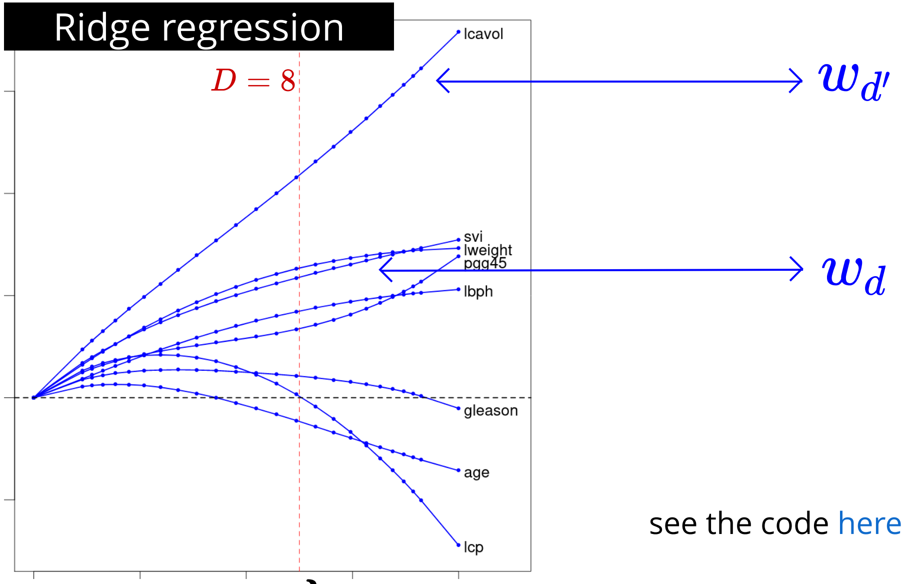
regularization path shows how $\{w_d\}$ change as we change λ

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

Example

$D = 8$





decreasing regularization coef. λ

see the code here

red-line is the optimal λ from cross-validation, for lasso the model uses only 3 of the 8 features

$\Rightarrow$ lasso results in sparse models

optional

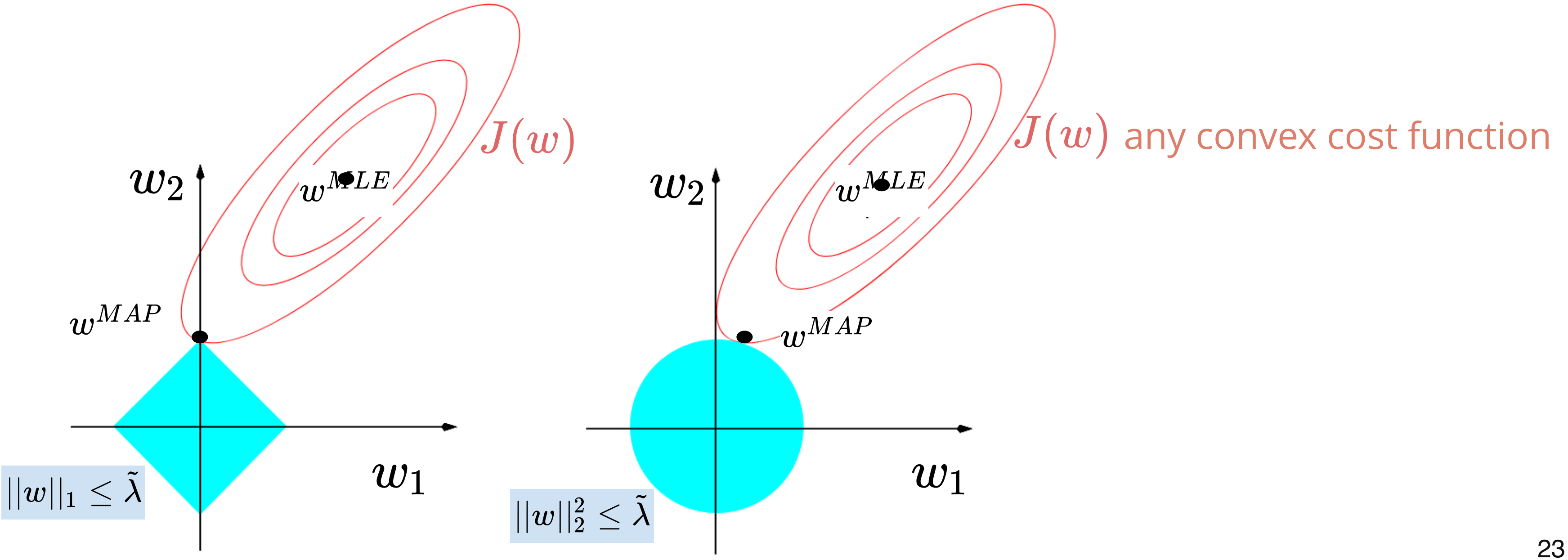
L_1 vs L_2 regularization

$\min_w J(w) + \lambda ||w||_p^p$

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

figures below show the constraint and the isocontours of $J(w)$

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

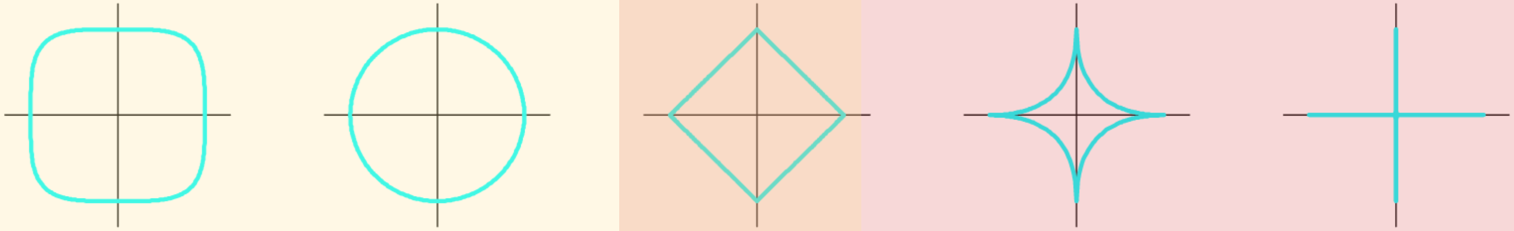


optional

Subset selection

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

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



$\left(\sum_d w_d^4\right)^{1/4}$ $\left(\sum_d w_d^2\right)^{\frac{1}{2}}$ $\sum_d |w_d|$ $\left(\sum_d |w_d|^{\frac{1}{2}}\right)^2$ $\left(\sum_d |w_d|^{\frac{1}{10}}\right)^{10}$

closer to **0-norm** → L_0 norm

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

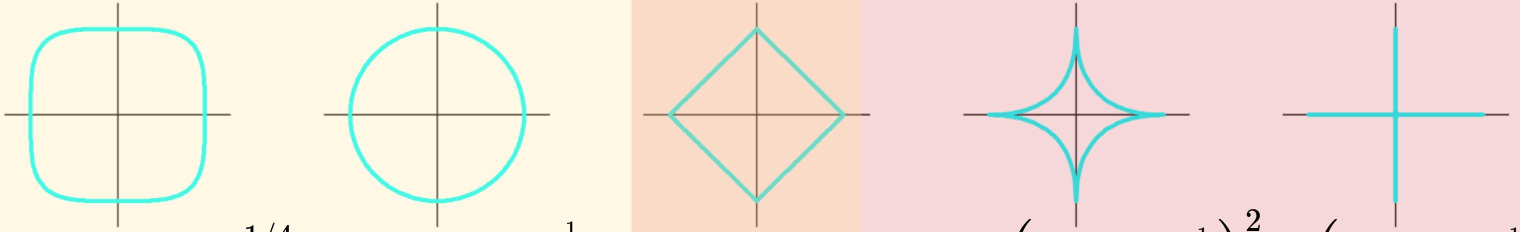
$$J(w) + \lambda ||w||_0 = J(w) + \lambda \sum_d \mathbb{I}(w_d \neq 0)$$

enforces a penalty of λ for each feature to be included in the model $\Rightarrow$ performs feature selection

Subset selection

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

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



$\left(\sum_d w_d^4\right)^{1/4}$ $\left(\sum_d w_d^2\right)^{\frac{1}{2}}$ $\sum_d |w_d|$ $\left(\sum_d |w_d|^{\frac{1}{2}}\right)^2$ $\left(\sum_d |w_d|^{\frac{1}{10}}\right)^{10}$

closer to **0-norm** → L_0 norm

L1 regularization is a viable alternative to L0 regularization

optimizing l_0 regularization is a difficult *combinatorial problem*: search over all 2^D subsets

Adding L_2 regularization

do not penalize the bias w_0

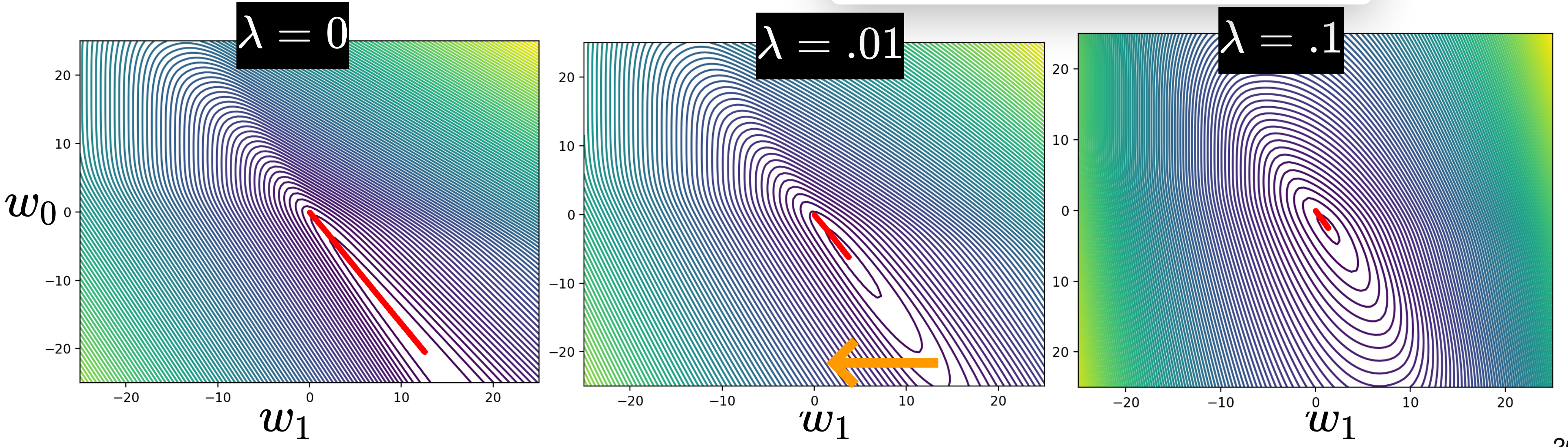
L2 penalty makes the optimization easier too!

note that the optimal w_1 **shrinks**

example for **logistic regression**

```
def gradient(x, y, w, lambdaa):
    N,D = x.shape
    yh = logistic(np.dot(x, w))
    grad = np.dot(x.T, yh - y) / N
    grad[1:] += lambdaa * w[1:]
    return grad
```

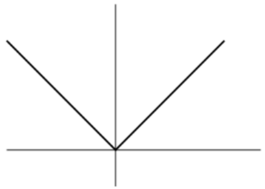
weight decay



similar pattern for **linear regression**, see example in the colab

optional

Subgderivatives



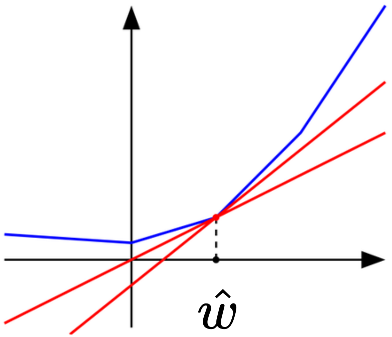
L1 penalty is no longer smooth or differentiable (at 0)

extend the notion of derivative to non-smooth functions

sub-differential is the set of all **sub-derivatives** at a point

$$\partial f(\hat{w}) = \left[\lim_{w \to \hat{w}^-} \frac{f(w) - f(\hat{w})}{w - \hat{w}}, \lim_{w \to \hat{w}^+} \frac{f(w) - f(\hat{w})}{w - \hat{w}}\right]$$

if $\boldsymbol{f}$ is differentiable at $\hat{w}$ then sub-differential has one member $\frac{d}{dw} f(\hat{w})$

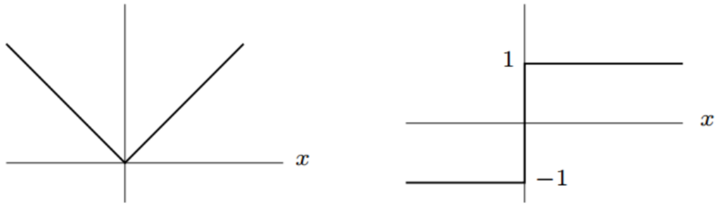


another expression for sub-differential

$$\partial f(\hat{w}) = \{g \in \mathbb{R} |\ f(w) > f(\hat{w}) + g(w - \hat{w})\}$$

Subgradient

example subdifferential for $f(w) = |w|$



$$\partial f(0) = [-1, 1]$$

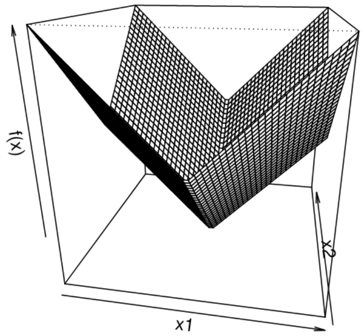
$$\partial f(w \neq 0) = \{\text{sign}(w)\}$$

recall, **gradient** was the vector of **partial derivatives**

subgradient is a vector of **sub-derivatives**

subdifferential for functions of multiple variables

$$\partial f(\hat{w}) = \{g \in \mathbb{R}^D | f(w) > f(\hat{w}) + g^\top (w - \hat{w})\}$$



we can use sub-gradient with diminishing step-size for optimization

image credit: G. Gordon

Adding L_1 regularization

L1-regularized *linear regression* has efficient solvers

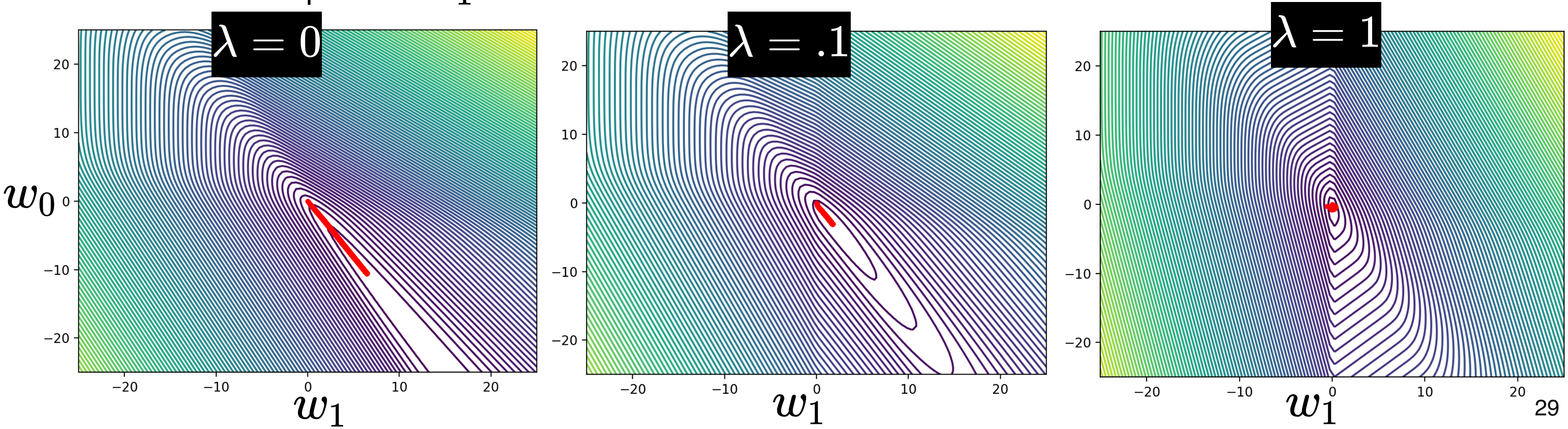
subgradient method for L1-regularized logistic regression

do not penalize the bias w_0

using diminishing learning rate

```
def gradient(x, y, w, lambdaa):
    N,D = x.shape
    yh = logistic(np.dot(x, w))
    grad = np.dot(x.T, yh - y) / N
    grad[1:] += lambdaa * np.sign(w[1:])
    return grad
```

note that the optimal w_1 **becomes 0**



Regularization serves many purposes

$$w^* = (X^\top X)^{-1} X^\top y$$

$D \times 1$ $D \times N$ $N \times D$ $N \times 1$

what if $X^\top X$ is **not invertible**?

add a small value to the diagonals, a.k.a. **regularize**

what if **linear fit is not the best**?

use nonlinear basis

How to avoid **overfitting** then? **regularize**

what if **we want a sparse model**?

do feature selection and only keep important parameters with **regularizing**

optional

Data normalization

what if we scale the input features, using different factors $\tilde{x}_d^{(n)} = \gamma_d x_d^{(n)} \forall d, n$

if we have no regularization: $\tilde{w}_d = \frac{1}{\gamma_d} w_d \forall d$

everything remains the same because: $||Xw - y||_2^2 = ||\tilde{X}\tilde{w} - y||_2^2$

with regularization: $||\tilde{w}||_2 \neq ||w||_2^2$ so the optimal **w** will be different!

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 $x_d^{(n)} \leftarrow \frac{x_d^{(n)} - \mu_d}{\sigma_d}$

we saw that this also helps with the optimization!

Summary

- complex models can overfit to training data
- regularization avoids this by penalizing model complexity
  - L1 & L2 regularization
  - probabilistic interpretation: different priors on weights
  - L1 produces sparse solutions (useful for feature selection)