DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 6 | Part 1

Ridge Regression

News

- Discussion worksheet solutions.

Recall: Regression with Basis Functions

- We can fit any function of the form:

$$H(\vec{x}; \vec{w}) = w_0 + w_1 \phi_1(\vec{x}) + w_2 \phi_2(\vec{x}) + \ldots + w_k \phi_k(\vec{x})$$

- $\phi_i(\vec{x}) : \mathbb{R}^d \to \mathbb{R}$ is called a **basis function**.

Procedure

1. Define $\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \phi_2(\vec{x}), \ldots, \phi_k(\vec{x}))^T$

2. Form $n \times k$ **design matrix**:

$$\Phi = \begin{pmatrix} \text{Aug}(\phi(\vec{x}^{(1)})) & \longrightarrow \\ \text{Aug}(\phi(\vec{x}^{(2)})) & \longrightarrow \\ \vdots & \vdots \\ \text{Aug}(\phi(\vec{x}^{(n)})) & \longrightarrow \end{pmatrix} = \begin{pmatrix} \phi_1(\vec{x}^{(1)}) & \phi_2(\vec{x}^{(1)}) & \ldots & \phi_k(\vec{x}^{(1)}) \\ \phi_1(\vec{x}^{(2)}) & \phi_2(\vec{x}^{(2)}) & \ldots & \phi_k(\vec{x}^{(2)}) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(\vec{x}^{(n)}) & \phi_2(\vec{x}^{(n)}) & \ldots & \phi_k(\vec{x}^{(n)}) \end{pmatrix}$$

3. Solve the **normal equations**:

$$\vec{w}^* = (\Phi^T \Phi)^{-1} \Phi^T \vec{y}$$

Example: Polynomial Curve Fitting

- Fit a function of the form:

$$H(x; \vec{w}) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

- Use basis functions:

$$\phi_0(x) = 1 \qquad \phi_1(x) = x \qquad \phi_2(x) = x^2 \qquad \phi_3(x) = x^3$$

Example: Polynomial Curve Fitting

- Design matrix becomes:

$$\Phi = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ \dots & \dots & \ddots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 \end{pmatrix}$$

Gaussian Basis Functions

- **Gaussians** make for useful basis functions.

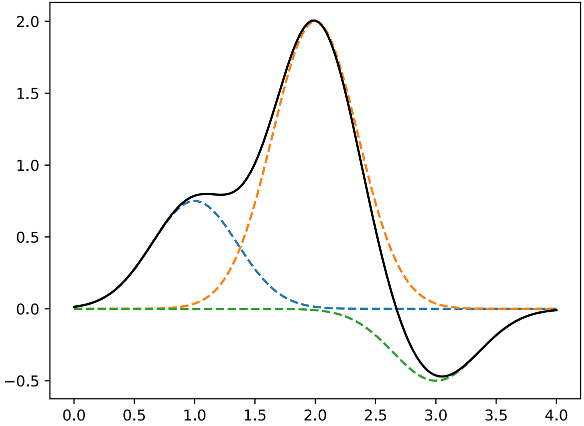
$$\phi_i(x) = \exp\left(-\frac{(x - \mu_i)^2}{\sigma_i^2}\right)$$

- Must specify[1] **center** μ_i and **width** σ_i for each Gaussian basis function.

[1]You pick these; they are not learned!

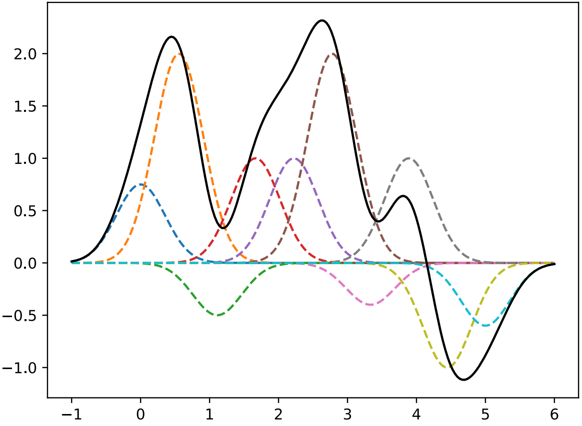
Example: $k = 3$

- A function of the form: $H(x) = w_1\phi_1(x) + w_2\phi_2(x) + w_3\phi_3(x)$, using 3 Gaussian basis functions.



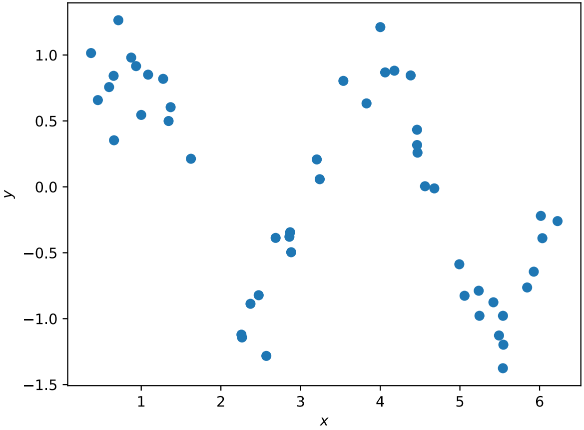
Example: $k = 10$

- The more basis functions, the more complex H can be.



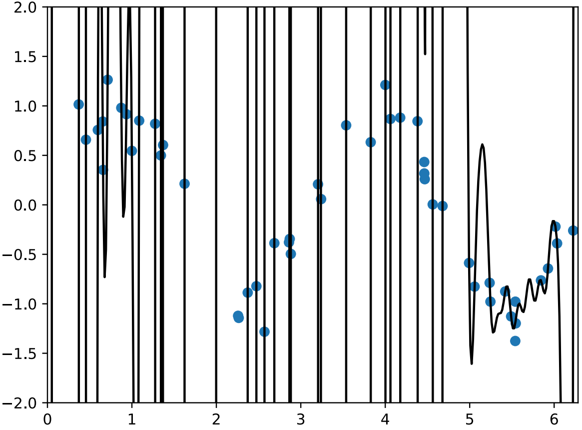
Demo: Sinusoidal Data

- Fit curve to 50 noisy data points.
- Use $k = 50$ Gaussian basis functions.



Result

- **Overfitting!**



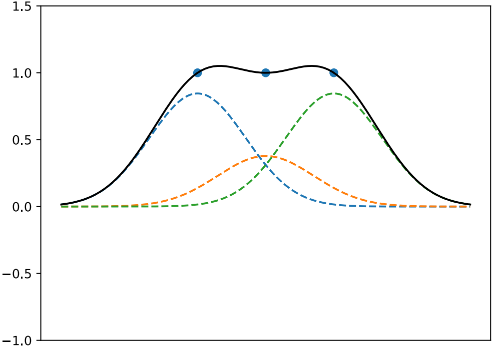
Controlling Model Complexity

- Model is too complex.
- Can decrease complexity by reducing number of basis functions.
- Another way: **regularization.**

Complexity and $\vec{w}$

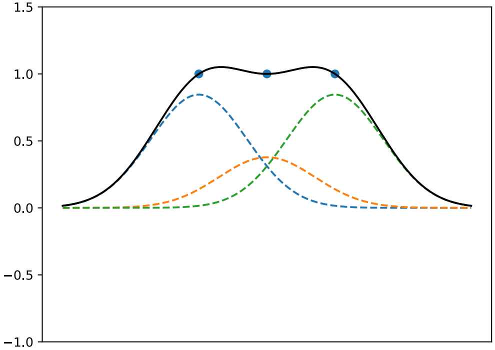
- Consider fitting 3 points with $k = 3$:

$$w_1 \phi_1(\vec{x}) + w_2 \phi_2(\vec{x}) + w_3 \phi_3(\vec{x})$$

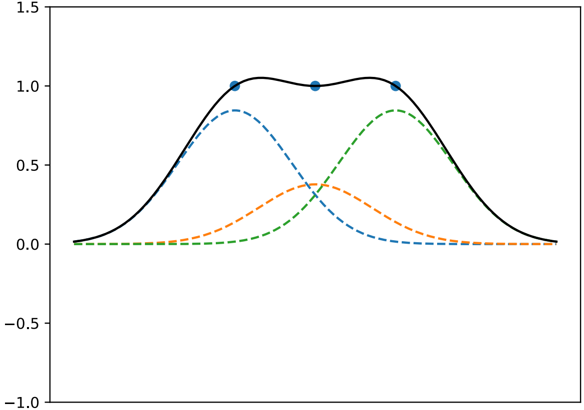


Exercise

What will happen to w_1, w_2, w_3 as the middle point is shifted down towards zero?



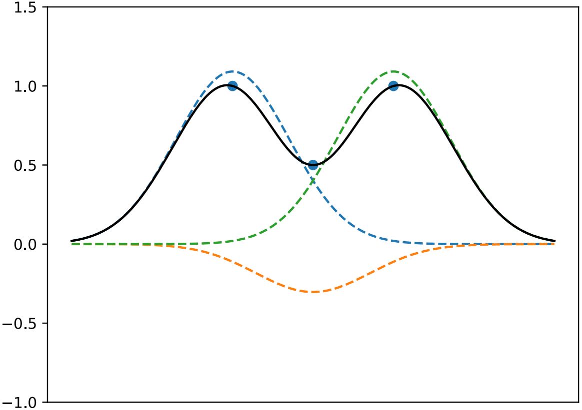
Solution



w = [0.85 0.38 0.85]

$\|\vec{w}\| = 1.25$

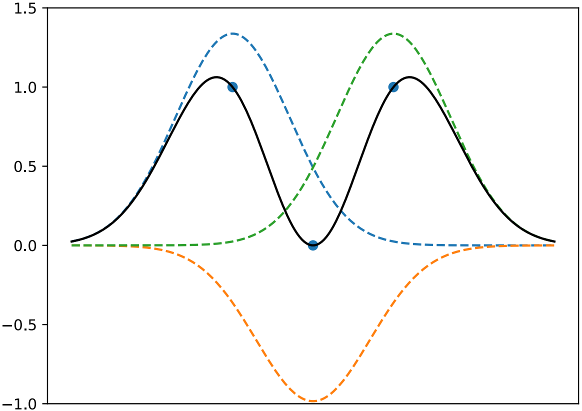
Solution



`w = [ 1.09 -0.3 1.09]`

$\|\vec{w}\| = 1.57$

Solution



w = [1.34 -0.98 1.34]

$\|\vec{w}\| = 2.13$

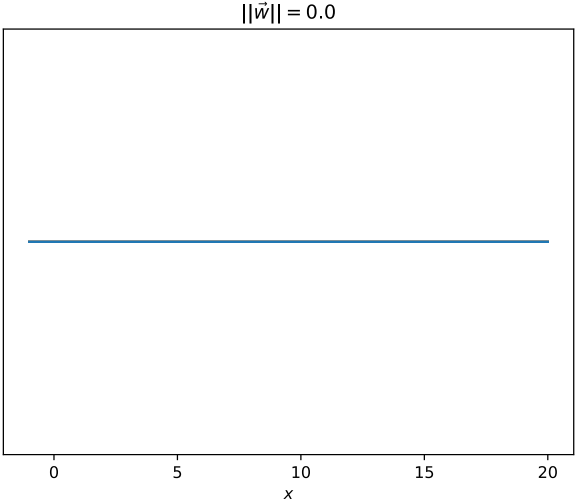
Observations

- As the middle point moves down, H becomes more complex.
- The weights grow in magnitude.
- $\|\vec{w}\|$ grows.
- **Idea:** $\|\vec{w}\|$ measures **complexity** of H.

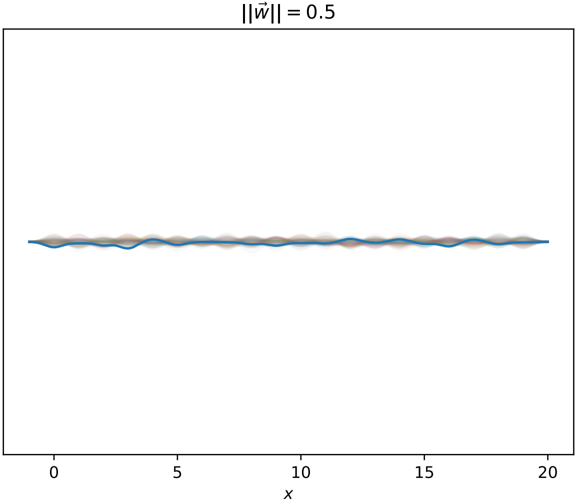
Experiment

- Consider model with $k = 20$ Gaussian basis functions.
- Generate 100 random parameter vectors $\vec{w}$.
- Plot overlapping; observe complexity.

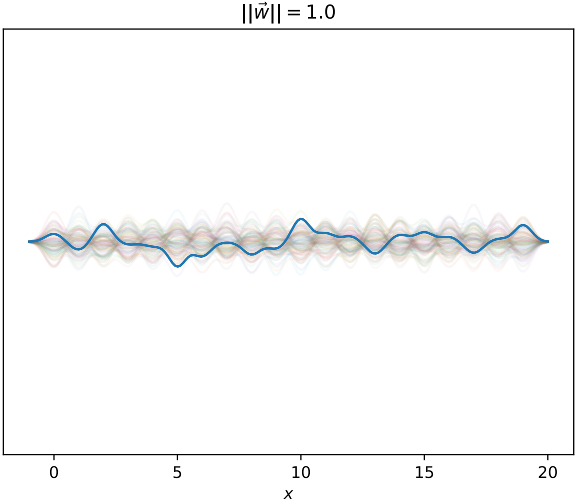
Experiment



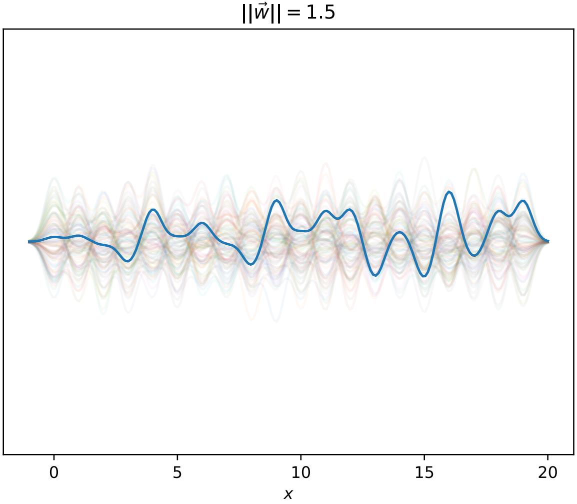
Experiment



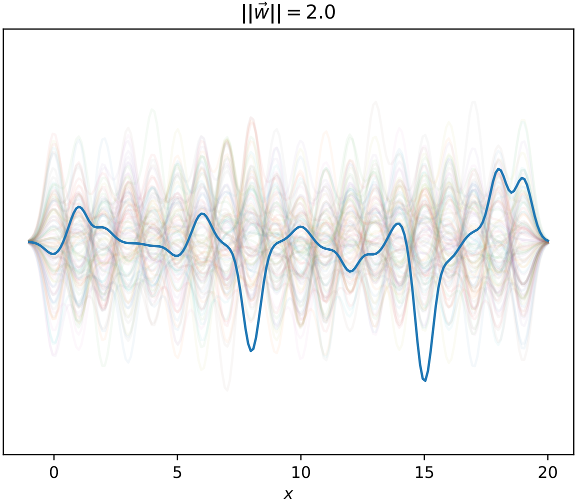
Experiment



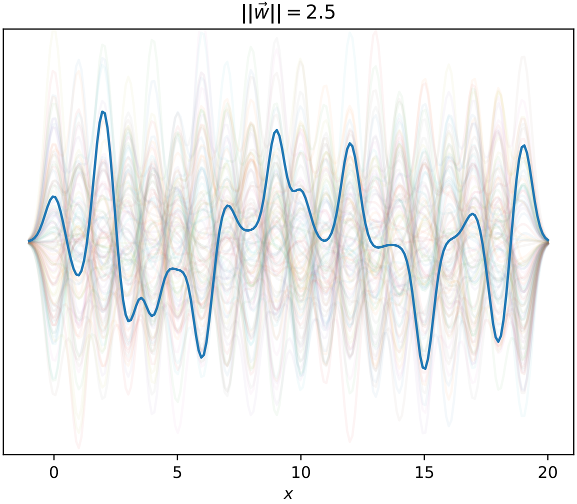
Experiment



Experiment



Experiment



Conclusion

- $\|\vec{w}\|$ is a proxy for model complexity.
  - The larger $\|w\|$, the more complex the model may be.

- **Idea:** find a model with
  - small mean squared error on the training data;
  - but also small $\|\vec{w}\|$

Recall: Least Squares Regression

- In **least squares regression**, we minimize the empirical **risk**:

$$
\begin{aligned}
R(\vec{w}) &= \frac{1}{n} \sum_{i=1}^{n} \left(H(\vec{x}^{(i)}) - y_i \right)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \phi(\vec{x}^{(i)}) - y_i \right)^2
\end{aligned}
$$

Regularized Least Squares

- **Idea:** penalize large $\|\vec{w}\|$ to control overfitting.

- **Goal:** Minimize the **regularized risk**:

$$\tilde{R}(\vec{w}) = \overbrace{\frac{1}{n}\sum_{i=1}^{n}\left(\vec{w}\cdot\phi(\vec{x}^{(i)}) - y_i\right)^2}^{\text{MSE}} + \lambda\|\vec{w}\|^2$$

- $\lambda\|\vec{w}\|^2$ is a **regularization term**.
  - "Tikhonov regularization"
  - λ controls "strength" of regularization.

Ridge Regression

- Least squares with $\|\vec{w}\|^2$ regularization is also known as **ridge regression**.

Why $\|\vec{w}\|^2$?

- We consider $\|\vec{w}\|^2$ instead of $\|\vec{w}\|$ because it will make the calculations cleaner.

Ridge Regression Solution

- **Goal:** Find $\vec{w}^*$ minimizing the **regularized risk**:

$$\frac{d}{dx} x^2 = 2x$$

$$\tilde{R}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \phi(\vec{x}^{(i)}) - y_i \right)^2 + \lambda \|\vec{w}\|^2$$

$$\frac{d}{d\vec{x}} \vec{x} \cdot \vec{x} = 2\vec{x}$$

- Recall:

$$\frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \phi(\vec{x}^{(i)}) - y_i \right)^2 = \frac{1}{n} \|\Phi \vec{w} - \vec{y}\|^2$$

- So:

$$\tilde{R}(\vec{w}) = \frac{1}{n} \|\Phi \vec{w} - \vec{y}\|^2 + \lambda \|\vec{w}\|^2$$

$\lambda I = \begin{pmatrix} \lambda & & 0 \\ & \lambda & \\ 0 & & \lambda \end{pmatrix}$

$\nabla_{\vec{w}} \tilde{R}$

Ridge Regression Solution

- **Strategy:** calculate $d\tilde{R}/d\vec{w}$, set to $\vec{0}$, solve.
- **Solution:** $\vec{w}^* = (\Phi^T \Phi + \cancel{\lambda I} \; n\lambda I)^{-1} \Phi^T \vec{y}$

  I is the identity matrix
- Compare this to solution of unregularized problem: $\vec{w}^* = (\Phi^T \Phi)^{-1} \Phi^T \vec{y}$

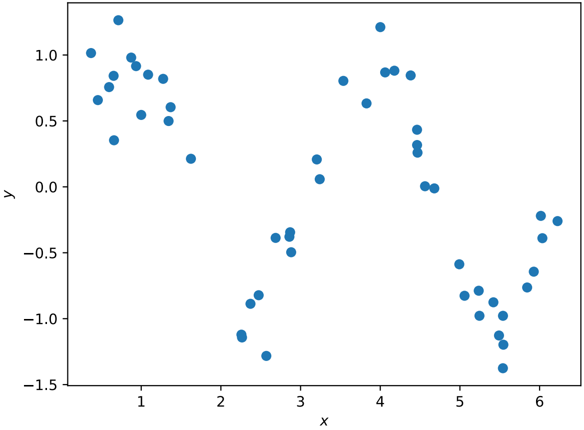
Interpretation

$$\vec{w}^* = (\Phi^T\Phi + \cancel{\lambda I} \xrightarrow{} n\lambda I)^{-1}\Phi^T\vec{y}$$

- Adds small number ~~λ~~ $n\lambda$ to diagonal of $\Phi^T\Phi$
- Improves condition number of $\Phi^T\Phi +$ ~~λI~~ $n\lambda I$
  - Helpful when multicollinearity exists

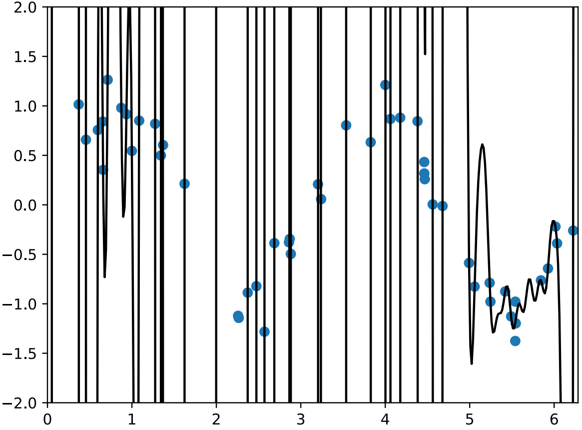
Demo: Sinusoidal Data

- Fit curve to 50 noisy data points.
- Use k = 50 Gaussian basis functions.

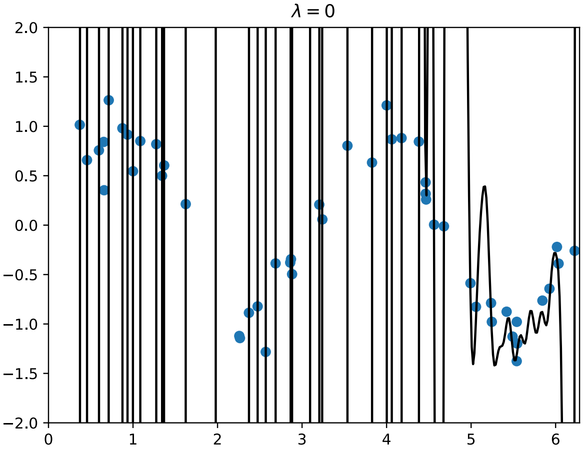


Result: no regularization

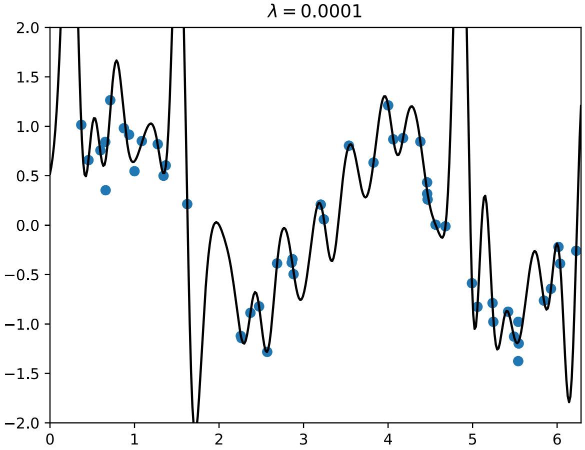
- **Overfitting!**



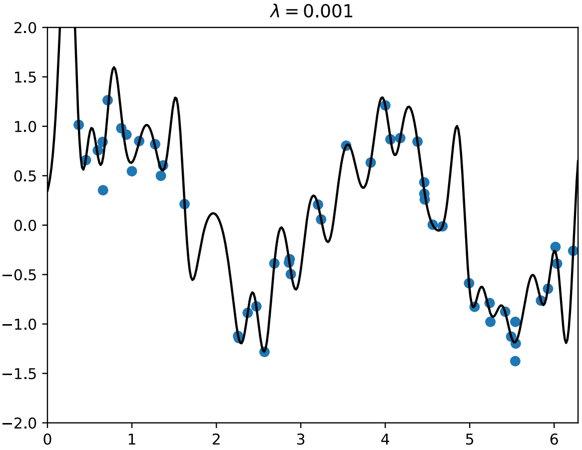
Result: regularization



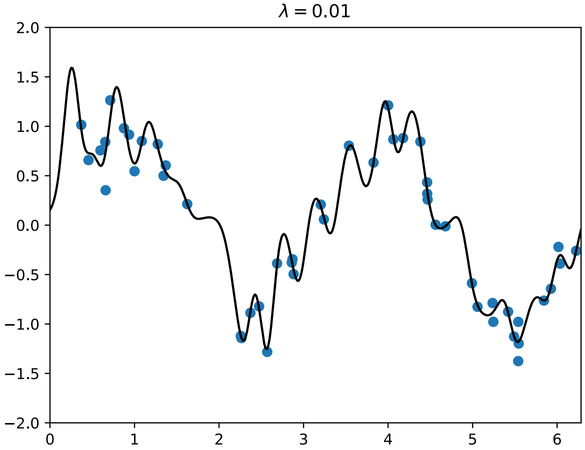
Result: regularization



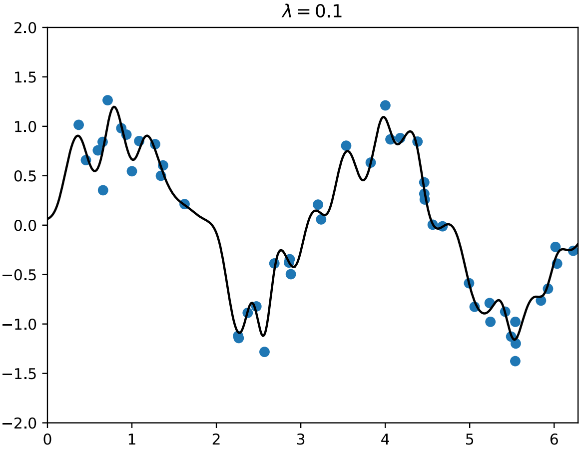
Result: regularization



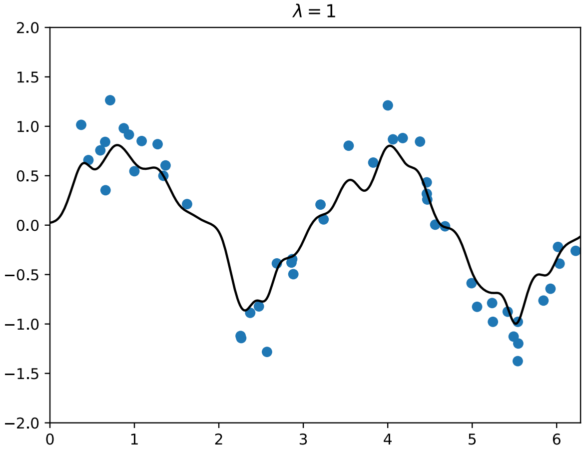
Result: regularization



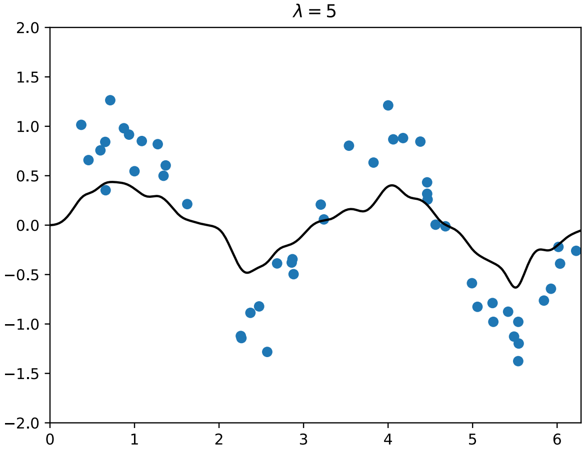
Result: regularization



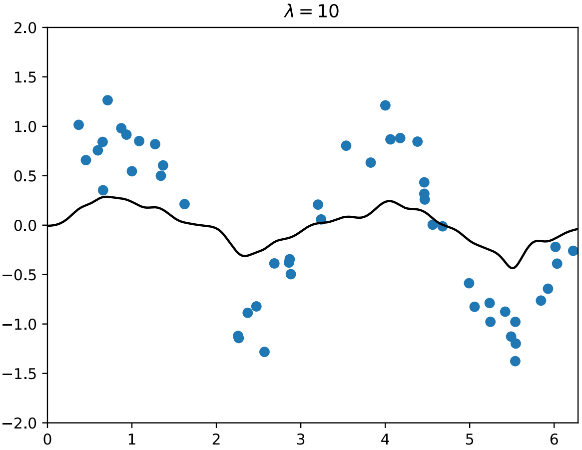
Result: regularization



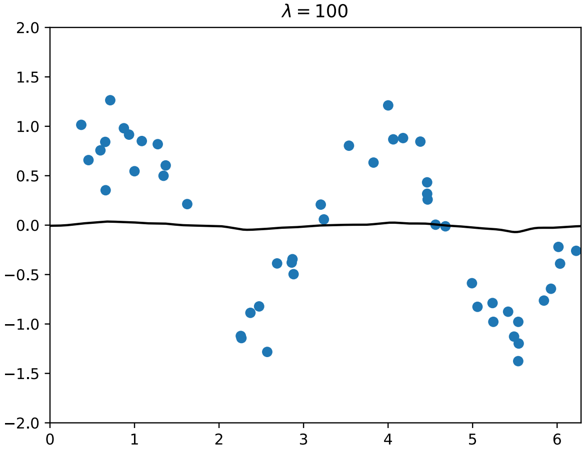
Result: regularization



Result: regularization



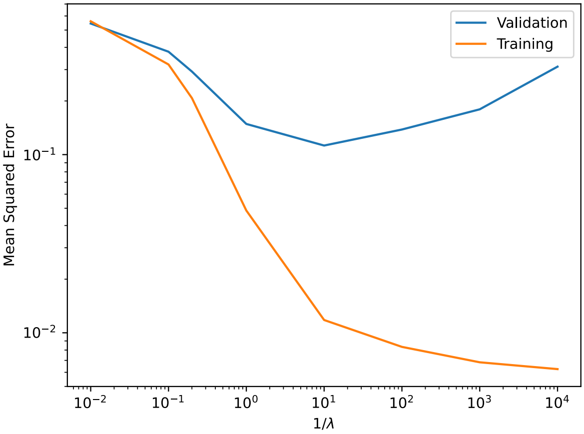
Result: regularization



Picking λ

- λ controls strength of penalty
  - Larger λ: penalize complexity more
  - Smaller λ: allow more complexity

- To choose, use **cross-validation**.


Validation
Training
Mean Squared Error
10^{-1}
10^{-2}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
$1/\lambda$

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Probabilistic Modeling & Machine Learning

Lecture 6 | Part 2

The LASSO

$\|\vec{u}\| = \sqrt{u_1^2 + u_2^2 + \ldots + u_d^2}$

p norm regularization

- In the last section, we minimized:

$$\tilde{R}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \phi(\vec{x}^{(i)}) - y_i\right)^2 + \lambda \|\vec{w}\|^2$$

- What is special about $\|\vec{w}\|$?

p norms

- For any $p \in [0, \infty)$, the **p norm** of a vector $\vec{u}$ is defined as

$$\|\vec{u}\|_p = \left(\sum_{i=1}^{d} |u_i|^p\right)^{1/p}$$

Special Case: $p = 2$

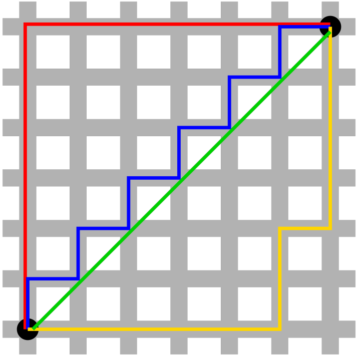
- When $p = 2$, we have the familiar **Euclidean norm**:

$$\|\vec{u}\|_2 = \left(\sum_{i=1}^{d} u_i^2 \right)^{1/2} = \|\vec{u}\|$$

Special Case: $p = 1$

- When $p = 1$, we have the "taxicab norm"

$$\|\vec{u}\|_1 = \sum_{i=1}^{d} |u_i|$$



1-norm Regularization

- Consider the 1-norm regularized risk:

$$\tilde{R}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \phi(\vec{x}^{(i)}) - y_i\right)^2 + \lambda \|\vec{w}\|_1$$

- Least squares regression with 1-norm regularization is called the **LASSO**.

Solving the LASSO

- No longer differentiable.
- No exact solution, unlike ridge regression.[2]
- Can solve with subgradient descent.

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[2] Except in special cases, such as orthonormal Φ

1-norm Regularization

- The 1-norm encourages **sparse** solutions.
  - That is, solutions where many entries of $\vec{w}$ are zero.

- **Interpretation:** feature selection.

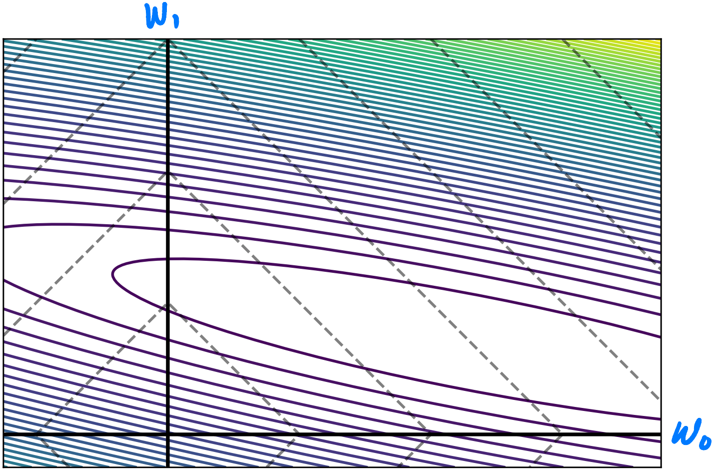
Example

- Randomly-generated data:

$$y = 3x_1 + 0.2x_2 - 4x_3 + \mathcal{N}(0, .2)$$

	w_1	w_2	w_3
Unreg.	2.33	-0.08	-4.77
2-norm	2.29	-0.10	-4.73
1-norm	2.72	0	-3.76

Why?



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Probabilistic Modeling & Machine Learning

Lecture 6 | Part 3

Regularized Risk Minimization

Regularized ERM

- We have seen regularization in the context of least squares regression.
- However, it is generally useful with other risks.
- E.g., hinge loss + 2-norm regularization = soft-SVM

General Regularization

- Let $R(\vec{w})$ be a risk function.
- Let $\rho(\vec{w})$ be a regularization function.
- The regularized risk is:

$$\tilde{R}(\vec{w}) = R(\vec{w}) + \rho(\vec{w})$$

- **Goal:** minimized regularized empirical risk.

Regularized Linear Models

Loss	Regularization	Name
square	2-norm	ridge regression
square	1-norm	LASSO
square	1-norm + 2-norm	elastic net
hinge	2-norm	soft-SVM