

DSC 140A

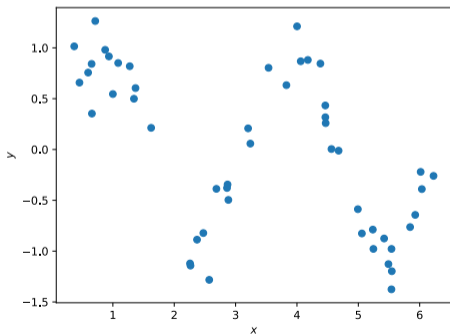
Probabilistic Modeling & Machine Learning

Lecture 8 | Part 1

Model Complexity and Regularization

Linear Regression, Non-linear Trends

- ▶ We can use least squares regression to fit non-linear patterns.



Recall: Regression with Basis Functions

- ▶ We can fit any function of the form:

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

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

Procedure

1. Define $\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \phi_2(\vec{x}), \dots, \phi_k(\vec{x}))^T$
2. Form $n \times k$ **design matrix**:

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

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:

$$H(x; \vec{w}) = w_0 + w_1x + w_2x^2 + w_3x^3$$

- ▶ Use basis functions:

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

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.

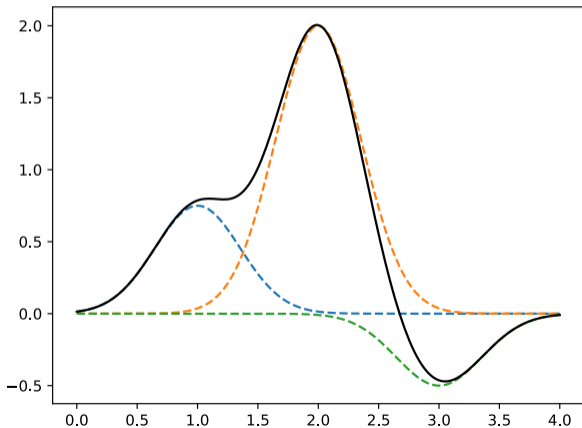
$$\phi_i(x) = \exp\left(-\frac{(x - \mu_i)^2}{\sigma_i^2}\right)$$

- ▶ Must specify¹ **center** μ_i and **width** σ_i for each Gaussian basis function.

¹You pick these; they are not learned!

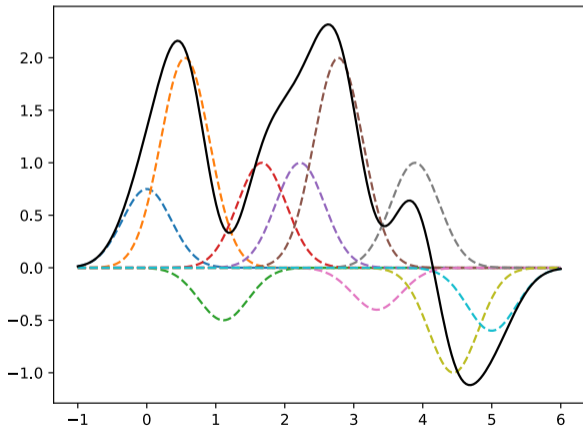
Example: $k = 3$

- ▶ 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.



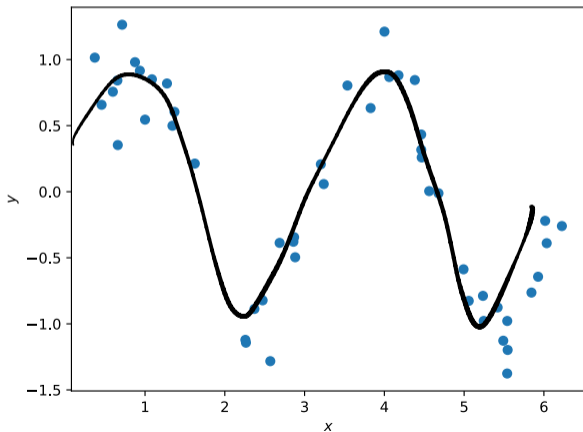
Example: $k = 10$

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



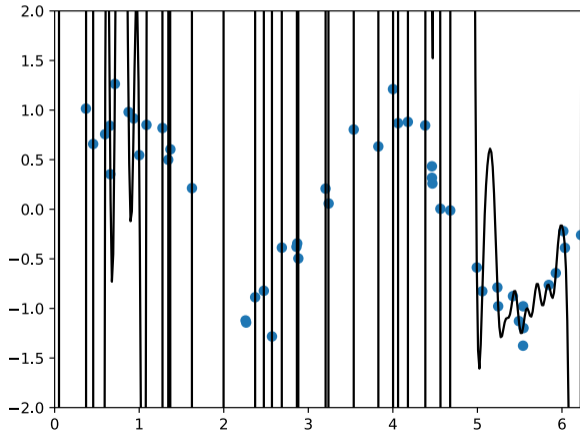
Demo: Sinusoidal Data

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



Result

► **Overfitting!**



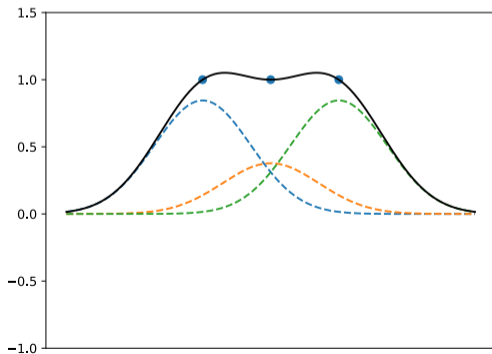
Today's Problem

- ▶ We sometimes want to fit complex models.
- ▶ **Overfitting** can occur when model is too complex.
- ▶ Can decrease complexity by reducing number of basis functions.
- ▶ Another way: **regularization.**

Complexity and \vec{w}

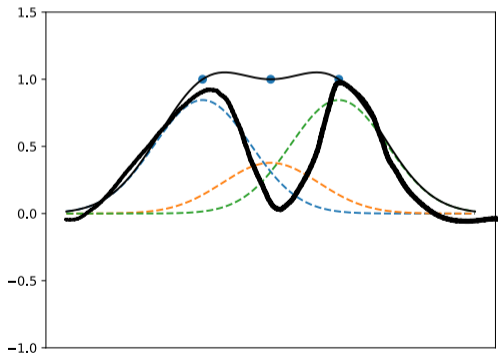
- ▶ Consider fitting 3 points with $k = 3$:

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

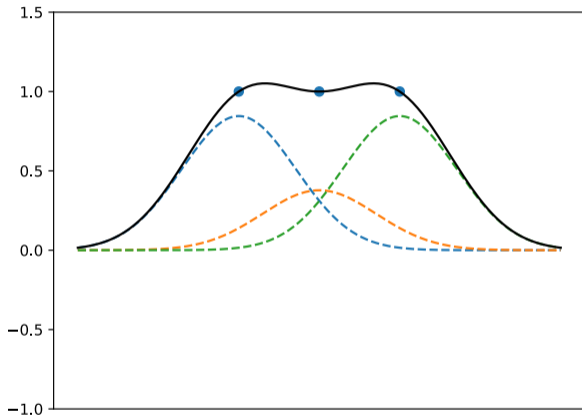


Exercise

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

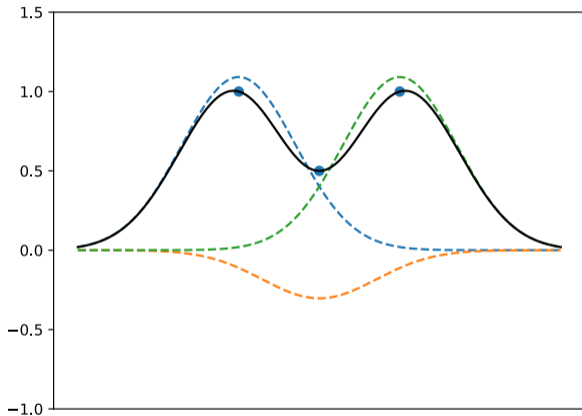


Solution



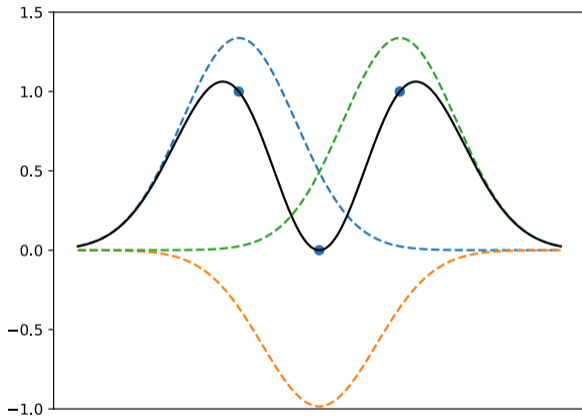
$$w = [0.85 \ 0.38 \ 0.85]$$
$$\|\vec{w}\| = 1.25$$

Solution



$$w = [1.09 \quad -0.3 \quad 1.09]$$
$$\|\vec{w}\| = 1.57$$

Solution



$$w = [1.34 \quad -0.98 \quad 1.34]$$
$$\|\vec{w}\| = 2.13$$

Observations

- ▶ As the middle point moves down, H becomes more “complex”.
- ▶ The weights grow in magnitude: $\|\vec{w}\|$ increases.
- ▶ **Idea:** $\|\vec{w}\|$ measures **complexity** of H .
 - ▶ Think: the larger $\|\vec{w}\|$ is, the more complex H may be.

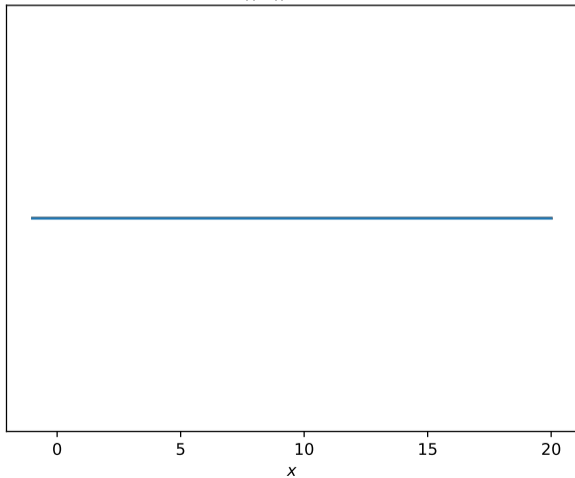
$$H(x) = w_1 \varphi_1(x) + w_2 \varphi_2(x) + \dots + w_{20} \varphi_{20}(x)$$

Experiment

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

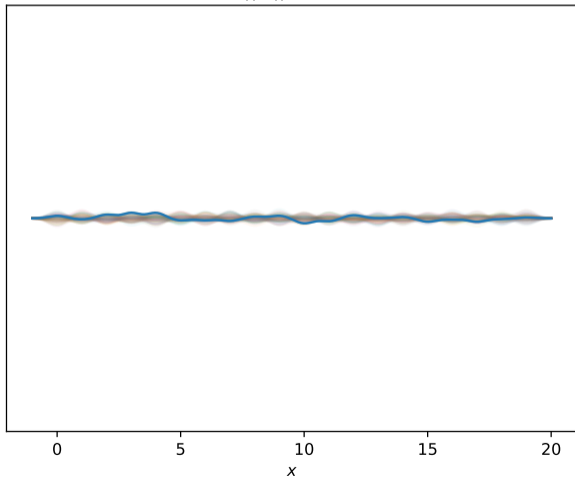
Experiment

$$\|\vec{w}\| = 0.0$$



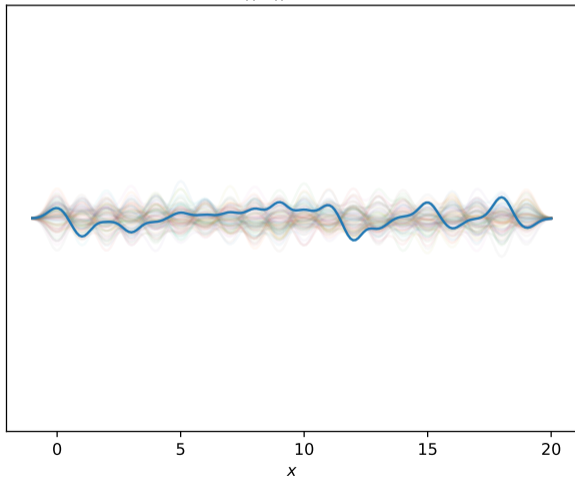
Experiment

$$\|\vec{w}\| = 0.5$$



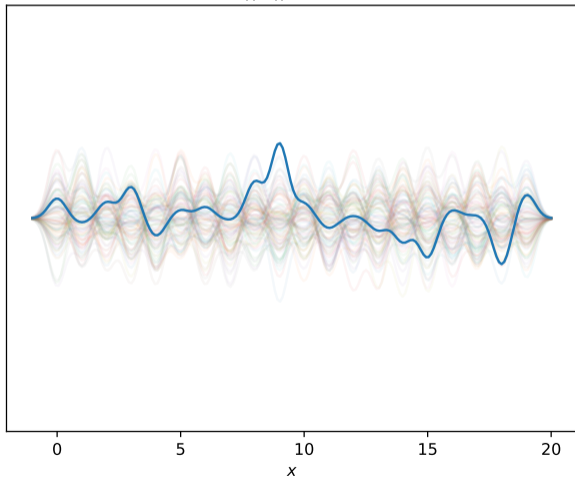
Experiment

$$\|\vec{w}\| = 1.0$$



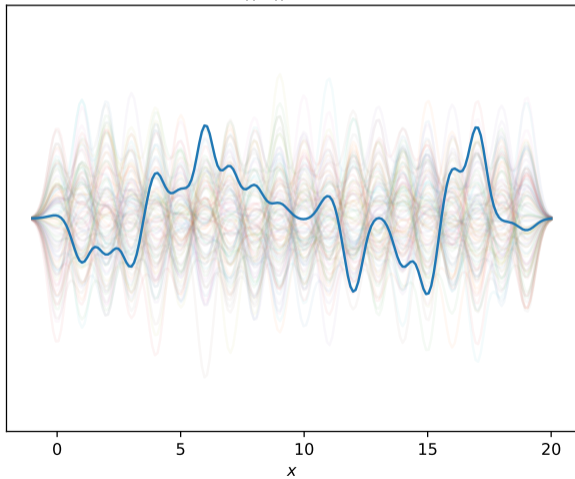
Experiment

$$\|\vec{w}\| = 1.5$$



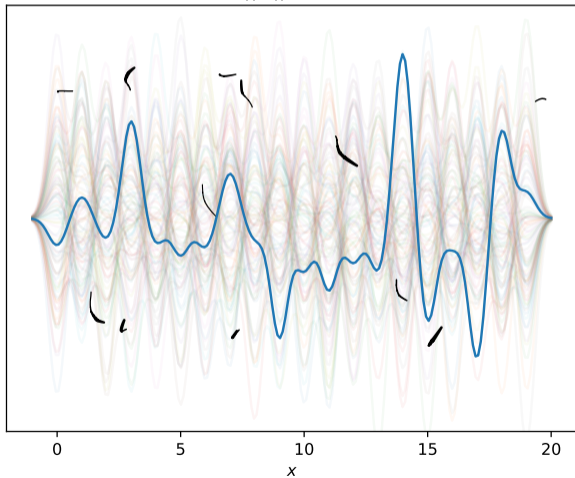
Experiment

$$\|\vec{w}\| = 2.0$$



Experiment

$$\|\vec{w}\| = 2.5$$



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 risk on the data;
 - ▶ but also small $\|\vec{w}\|$

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Probabilistic Modeling & Machine Learning

Lecture 8 | Part 2

Regularized Least Squares

Recall: Least Squares Regression

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

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

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

Regularized Least Squares

- ▶ **Idea:** penalize large $\|\vec{w}\|$ to control overfitting.
- ▶ **Goal:** Minimize the **regularized risk**:

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

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

Ridge Regression

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

- ▶ Least squares with $\|w\|^2$ 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

- ▶ Remember, with the unregularized problem, the least squares solution was:

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

- ▶ Now that we've regularized the risk, this is no longer the solution!

Ridge Regression Solution

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

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

- ▶ Recall:

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

- ▶ So:

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

Ridge Regression Solution

- ▶ **Strategy:** calculate $d\tilde{R}/d\vec{w}$, set to $\vec{0}$, solve.

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

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

$$\begin{pmatrix} n\lambda & & & \\ & n\lambda & & \\ & & & 0 \\ & & 0 & n\lambda \end{pmatrix}$$

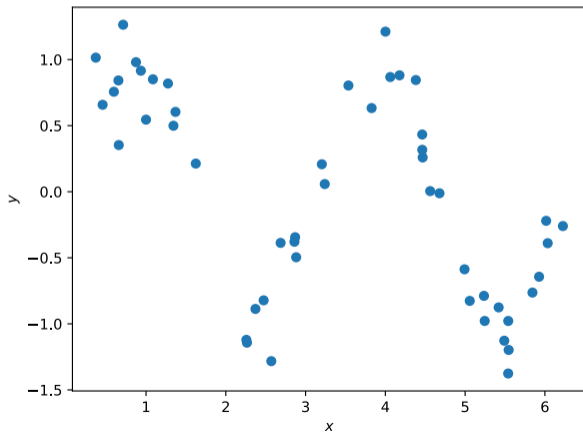
Interpretation

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

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

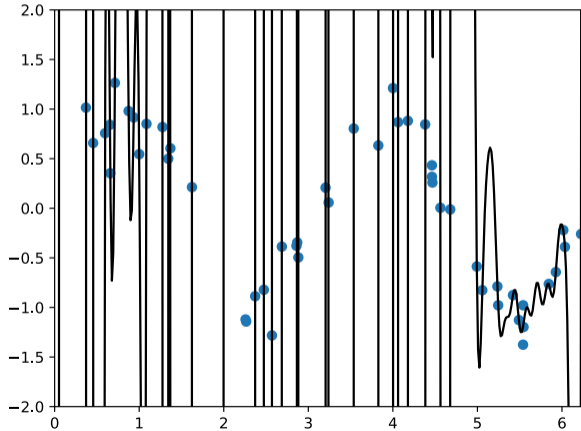
Demo: Sinusoidal Data

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

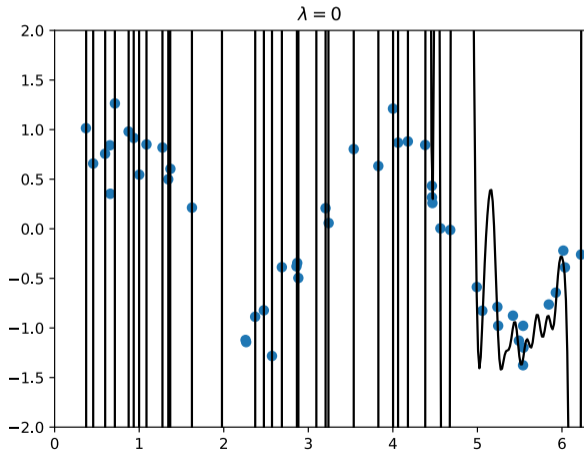


Result: no regularization

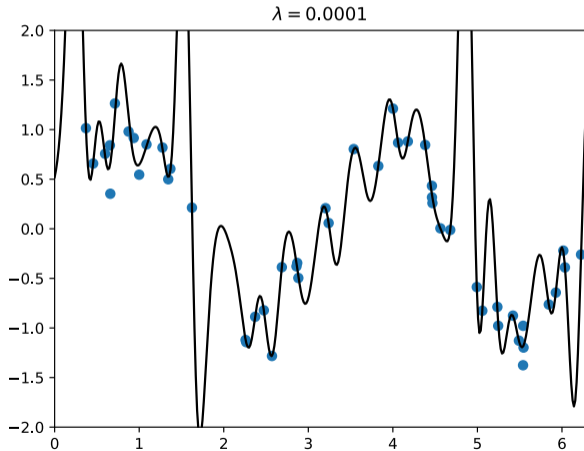
► **Overfitting!**



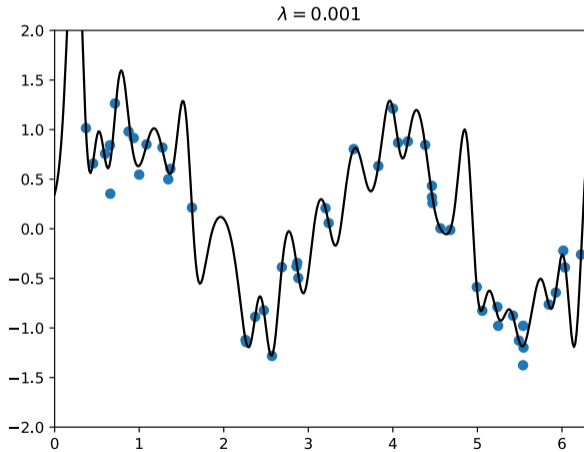
Result: regularization



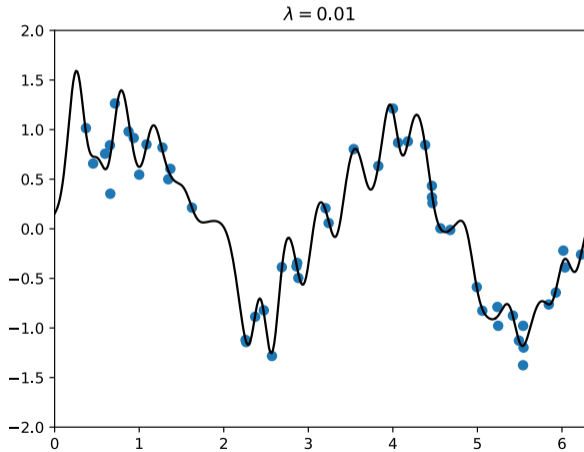
Result: regularization



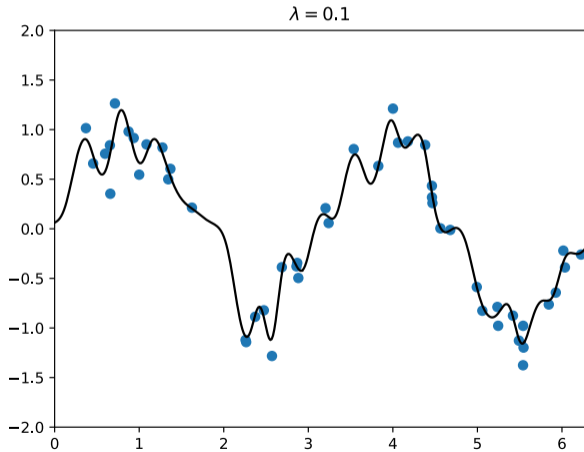
Result: regularization



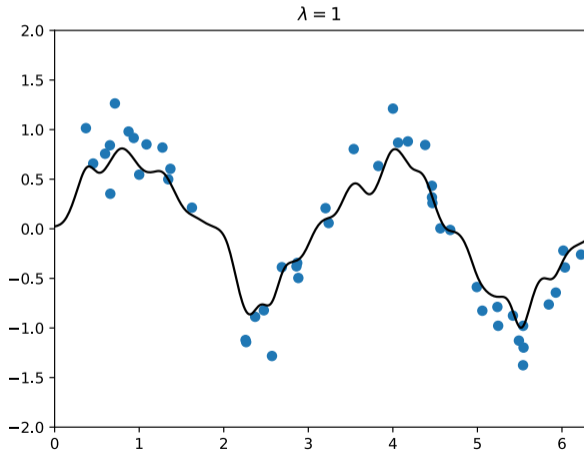
Result: regularization



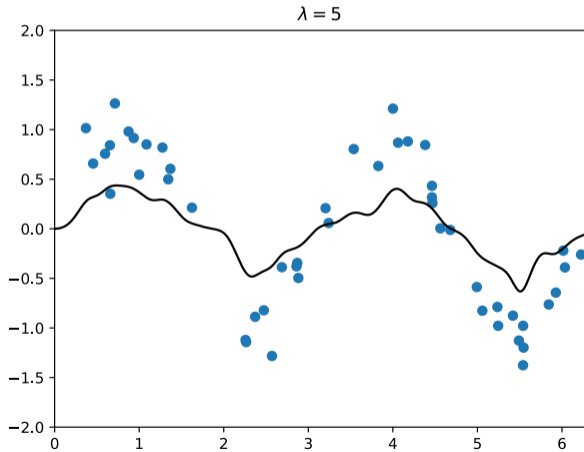
Result: regularization



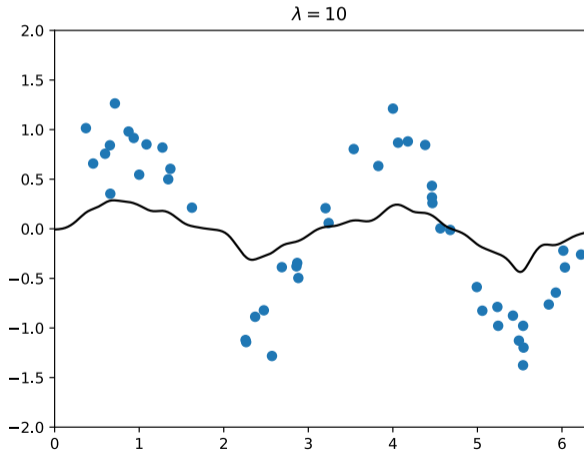
Result: regularization



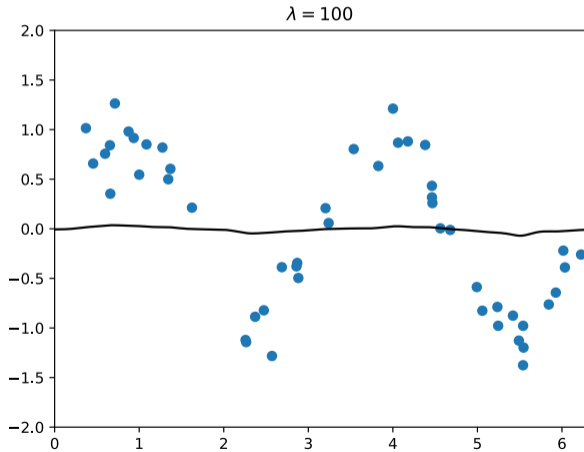
Result: regularization



Result: regularization

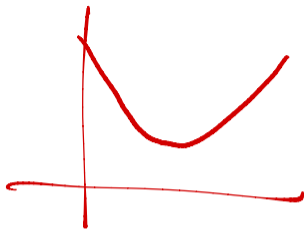


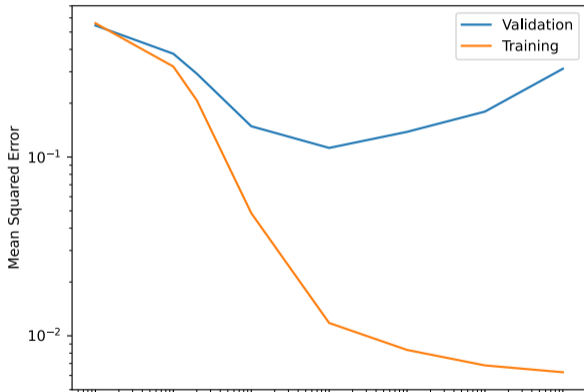
Result: regularization



Picking λ

- ▶ λ controls strength of penalty
 - ▶ Larger λ : penalize complexity more
 - ▶ Smaller λ : allow more complexity
- ▶ To choose, use **cross-validation**.





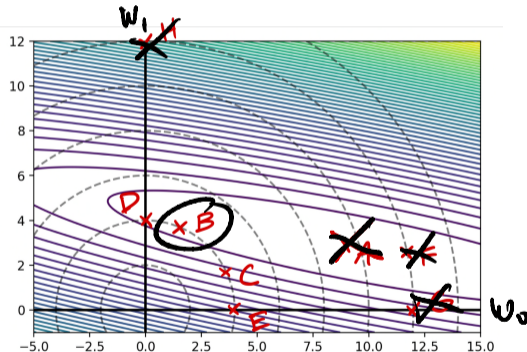
simple

complexity

complex

Exercise

Shown below are the contours of the unregularized empirical risk, $R(\vec{w})$. The dashed lines show places where $\|\vec{w}\|_2$ is 2, 4, 6, etc.



Which of the marked points could be a minimizer of the regularized risk, $\tilde{R}(\vec{w}) = R(\vec{w}) + \lambda \|\vec{w}\|_2^2$, where $\lambda > 0$?

Main Idea

Regularization trades an **increase** in risk for a **decrease** in complexity.

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Probabilistic Modeling & Machine Learning

Lecture 8 | Part 3

The LASSO

$$\sqrt{w_1^2 + w_2^2 + \dots + w_a^2}$$

p norm regularization

- ▶ In the last section, we minimized:

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

- ▶ 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

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

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

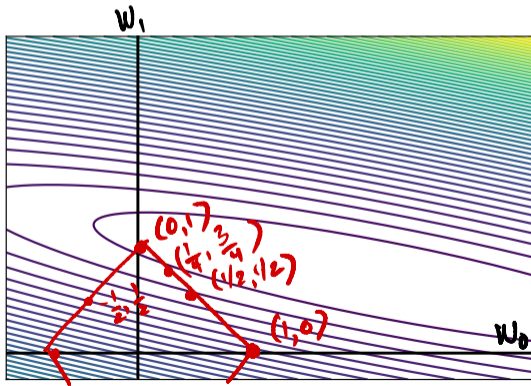
Special Case: $p = 2$

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

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

Exercise

Draw the “unit circle” for the 1-norm. That is, draw where $\|\vec{w}\|_1 = 1$.



$$\sum_i |w_i| = 1$$

$$\sum_i |w_i| = 2$$

$$|w_0| + |w_1| = 1$$

$$|w_0| + |w_1| = 2$$

⋮

1-norm Regularization

- ▶ Consider the 1-norm regularized risk:

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

- ▶ 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.

²Except 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.

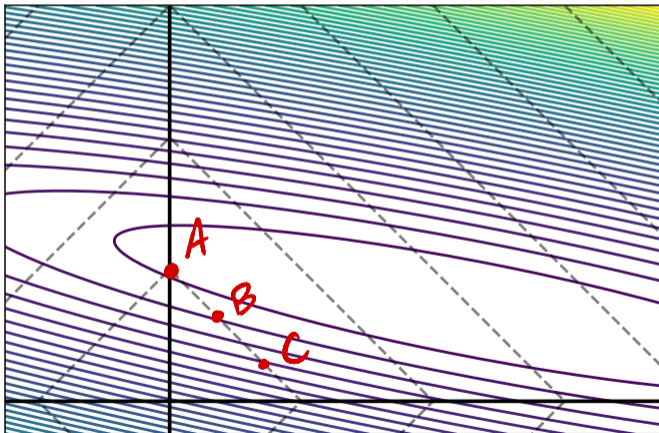
Example

- ▶ 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 8 | Part 4

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.

$$R(\vec{w}) + \lambda_1 \|\vec{w}\|_2^2 + \lambda_2 \|\vec{w}\|_1$$

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 |

Example

"Early Stopping"

