Regression II

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Solving the Least Squares using Normal Equation

• We call $\Phi^{\dagger} \equiv (\Phi^T \Phi)^{-1} \Phi^T$ pseudo-inverse (generalization of inverse to non-square matrix). See for a square invertable matrix Φ , we have $\Phi^{\dagger} = (\Phi^T \Phi)^{-1} \Phi^T = \Phi^{-1} (\Phi^T)^{-1} \Phi^T = \Phi^{-1}$

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$$= V_r \Sigma_r^{-2} V_r^T V_r \Sigma_r U_r^T \mathbf{t}$$

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• How about when $\sigma_i \to 0$?

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Adding regularization to control overfitting

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- Recall that the likelihood is given by

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• Beyesian Theorem that relates prior $p(\mathbf{w}|\lambda)$ to posterior $p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \beta, \lambda)$:

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• Using conjugate prior $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$, we can show that Posterior $p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \beta, \lambda) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$ where $\mathbf{m}_N = \mathbf{S}_N(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\mathbf{\Phi}^T\mathbf{t}), \ \mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \beta\mathbf{\Phi}^T\mathbf{\Phi}.$

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- This is your home work.

• When $p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I})$, we have $\mathbf{m}_N = \beta \mathbf{S}_N \mathbf{\Phi}^T \mathbf{t}$, $\mathbf{S}_N^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi}$

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- The maximum a posteriori (MAP) estimation is given by

$$\ln p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \beta, \lambda) = -\frac{\beta}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^T \phi(\mathbf{x}_n)\}^2 - \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \text{consts.}$$

$$\Rightarrow \arg\max_{\mathbf{w}} \ln p(\mathbf{w}|\mathbf{t}) = \arg\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{\Phi}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\alpha}{2\beta} \|\mathbf{w}\|_2^2$$

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{\Phi}\mathbf{w} - \mathbf{t}\|_{2}^{2} + \frac{\lambda}{2} \sum_{i=1}^{M} |\mathbf{w}_{j}|^{q} = \min_{\mathbf{w}} \frac{1}{2} \|\mathbf{\Phi}\mathbf{w} - \mathbf{t}\|_{2}^{2} + \frac{\lambda}{2} \|\mathbf{w}\|_{q}^{q}$$

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• Ridge regression (q=2)

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• When q < 1 the problem is non-convex (more sparsity).

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- How about 2D case?

Notes on Regularization

 From regularized problems to constrained problems. For convex problems, a regularized problem has an equivalent constrained problem.

$$\min_{x} f(x) + r(x) \Leftrightarrow \min_{x} f(x) \text{ s.t. } x \in \mathcal{S}$$

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Solving

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{\Phi}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2} \|\mathbf{w}\|_q^q$$

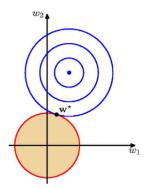
is equivalent to

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{\Phi}\mathbf{w} - \mathbf{t}\|_2^2 \text{ s.t. } \|\mathbf{w}\|_q^q \le z$$

Geometry Interpretation of Regularization

Ridge regression (q=2)

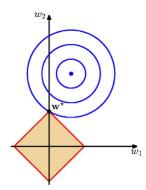
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Geometry Interpretation of Regularization

Lasso regression (q = 1)

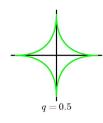
$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{\Phi}\mathbf{w} - \mathbf{t}\|_2^2 \text{ s.t. } \|\mathbf{w}\|_1 \le z$$

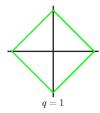


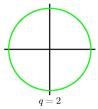
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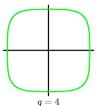
The more general ℓ_p regularizer:

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{\Phi}\mathbf{w} - \mathbf{t}\|_2^2 \text{ s.t. } \|\mathbf{w}\|_q^q \le z$$









Sparsity-Inducing Norms

- Lasso is commonly used for feature selection.
- Theory
 - http://www-stat.stanford.edu/~tibs/lasso.html
- Software
 - SLEP http://www.public.asu.edu/~jye02/Software/SLEP
 - FPC http://www-stat.stanford.edu/~tibs/lasso.html
 - L1_Ls http://www-stat.stanford.edu/~tibs/lasso.html

 If data points arrive sequentially, then the posterior distribution at any stage acts as the prior distribution for the subsequent data point, such that the new posterior distribution is updated sequentially.

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$$p(\mathbf{w}|\mathcal{D}; \alpha, \beta) = p(\mathbf{w}|\mathbf{t}, \mathbf{X}; \alpha, \beta) \propto p(\mathbf{t}|\mathbf{X}; \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

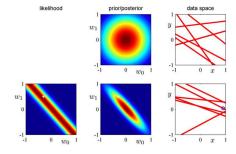
$$= \prod_{i=1}^{n} p(\mathbf{t}_{i}|\mathbf{x}_{i}; \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

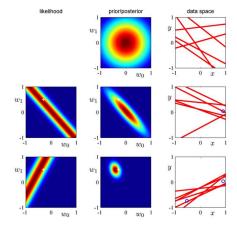
$$= \underbrace{p(\mathbf{t}_{n}|\mathbf{x}_{n}; \mathbf{w}, \beta)}_{\text{Likelihood}} \underbrace{\left[\prod_{i=1}^{n-1} p(\mathbf{t}_{i}|\mathbf{x}_{i}; \mathbf{w}, \beta)p(\mathbf{w}|\alpha)\right]}_{\text{Prior}}$$

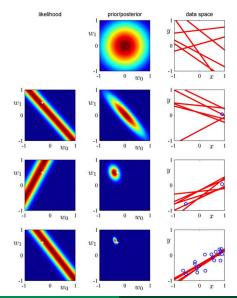












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$$= \int p(\hat{t}|\hat{\mathbf{x}}, \mathbf{w}; \beta) p(\mathbf{w}|\mathcal{D}; \alpha, \beta) d\mathbf{w}$$

where

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You will show that (in homework):

$$p(\hat{t}|\hat{\mathbf{x}};\mathcal{D},\alpha,\beta) = \mathcal{N}(\hat{t}|\mathbf{m}_N^T \boldsymbol{\phi}(\mathbf{x}),\sigma_N^2(\mathbf{x}))$$
 and variance $\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^T \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})$.

