MODEL FITTING II: RIDGE & TIKHONOV

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RECAP

* Linear regression!
* Ordinary least squares (OLS)
* Regularized regression
  * Priors on weights
  * Penalties on weights
  * Ad hoc metrics (early stopping)

RECAP

* L2 penalty = Gaussian prior = ridge

* L1 penalty = Laplacian prior = LASSO

TODO AY

* Analytic solutions to L2-regularized regression problems:

  * Ridge regression

  * Tikhonov regression

RIDGE REGRESSION

* Multivariate normal (MVN) prior on beta

* L2 penalty on beta

* Gradient descent w/ early stopping

RIDGE REGRESSI

\hat\beta = \underset{\beta}{\mbox{argmin}} \left[||Y-X\beta||_2^2 + \lambda ||\beta||_2^2 \right]

\hat\beta = \underset{\beta}

$$Y = X\beta + \epsilon$$

$$\hat{\beta} = \underset{\beta}{\text{argmin}} \left[||Y - X\beta||_2^2 + \lambda ||\beta||_2^2 \right]$$

ERROR or LOSS

PENALTY

RIDGE REGRESSION

$$\hat\beta = (X^\top X + \lambda I)^{-1} X^\top Y$$

$$\hat\beta = X^+_{ridge} Y$$

\hat\beta = (X^\top X + \lambda I)^{-1} X^\top Y

RIDGE REGRESSION

* Efficient solution with SVD

$$\hat{\beta} = (X^\top X + \lambda I)^{-1} X^\top Y$$

(SVD) $X = USV^\top$ $$D = \frac{S}{S^2 + \lambda^2}$$

$$\hat{\beta} = VDU^\top Y$$

\hat\beta = (X^\top X + \lambda I)^{-1} X^\top Y

D = \frac{S}{S^2 + \lambda^2}
\hat\beta = V D U^\top Y

RIDGE REGRESSION

* How to choose lambda?

* GCV - Generalized Cross Validation 👎

* Block-wise cross-validation 👍

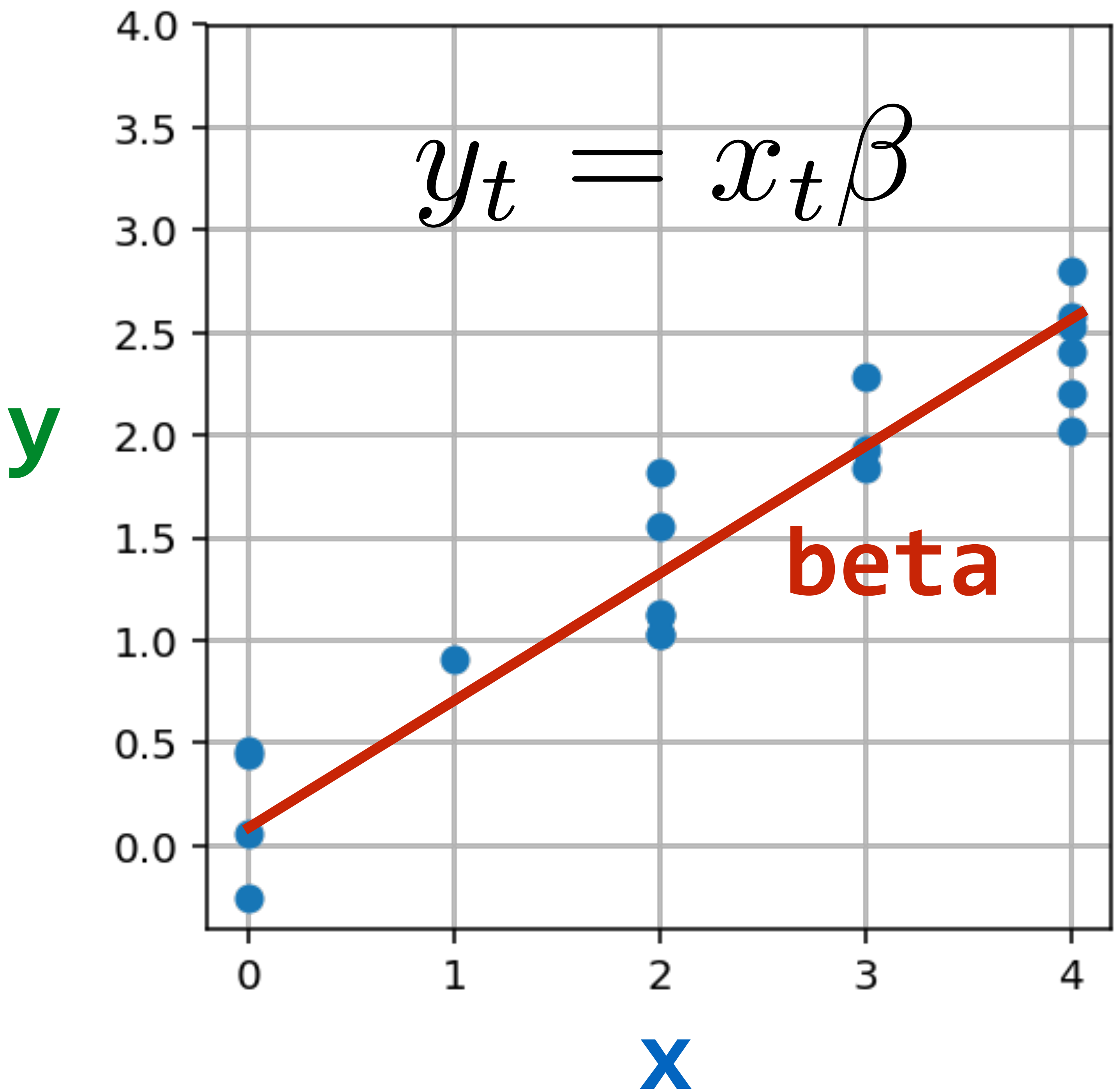
RIDGE REGRESSION

* Good implementation: scikit-learn

* Awesome implementation: http://github.com/alexhuth/ridge

Err(\beta) = \sum_{t=1}^T (y_t - x_t \beta)^2

1D EXAMPLE



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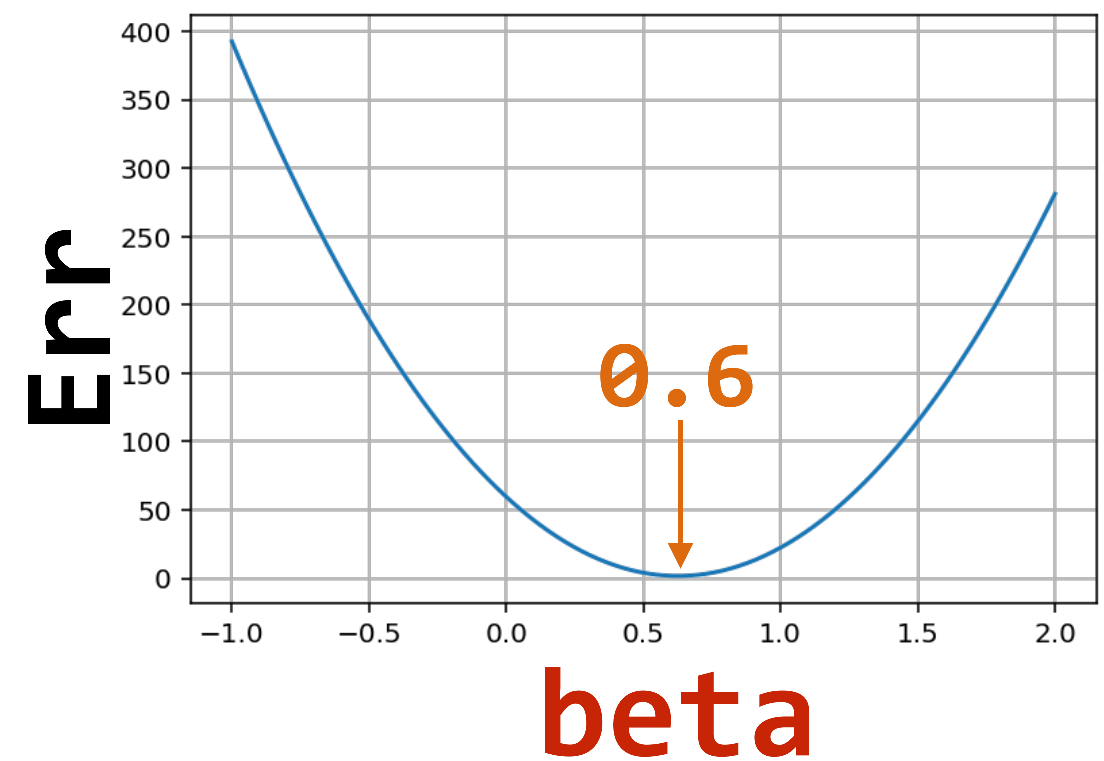

Err(\beta) = \sum_{t=1}^T (y_t - x_t \beta)^2 + \lambda \beta^2

1D EXAMPLE

L2 Regularization:
(as penalty)

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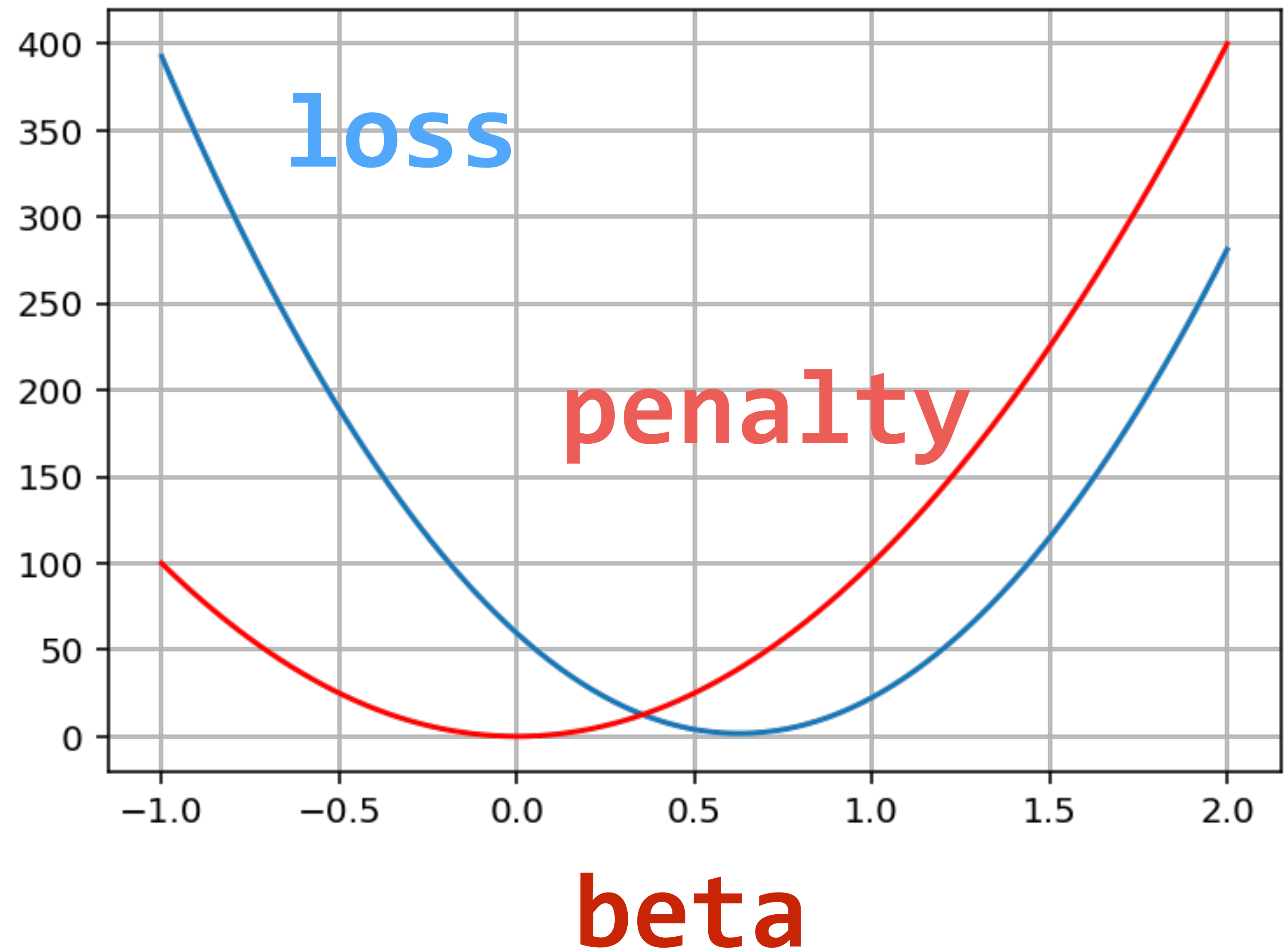

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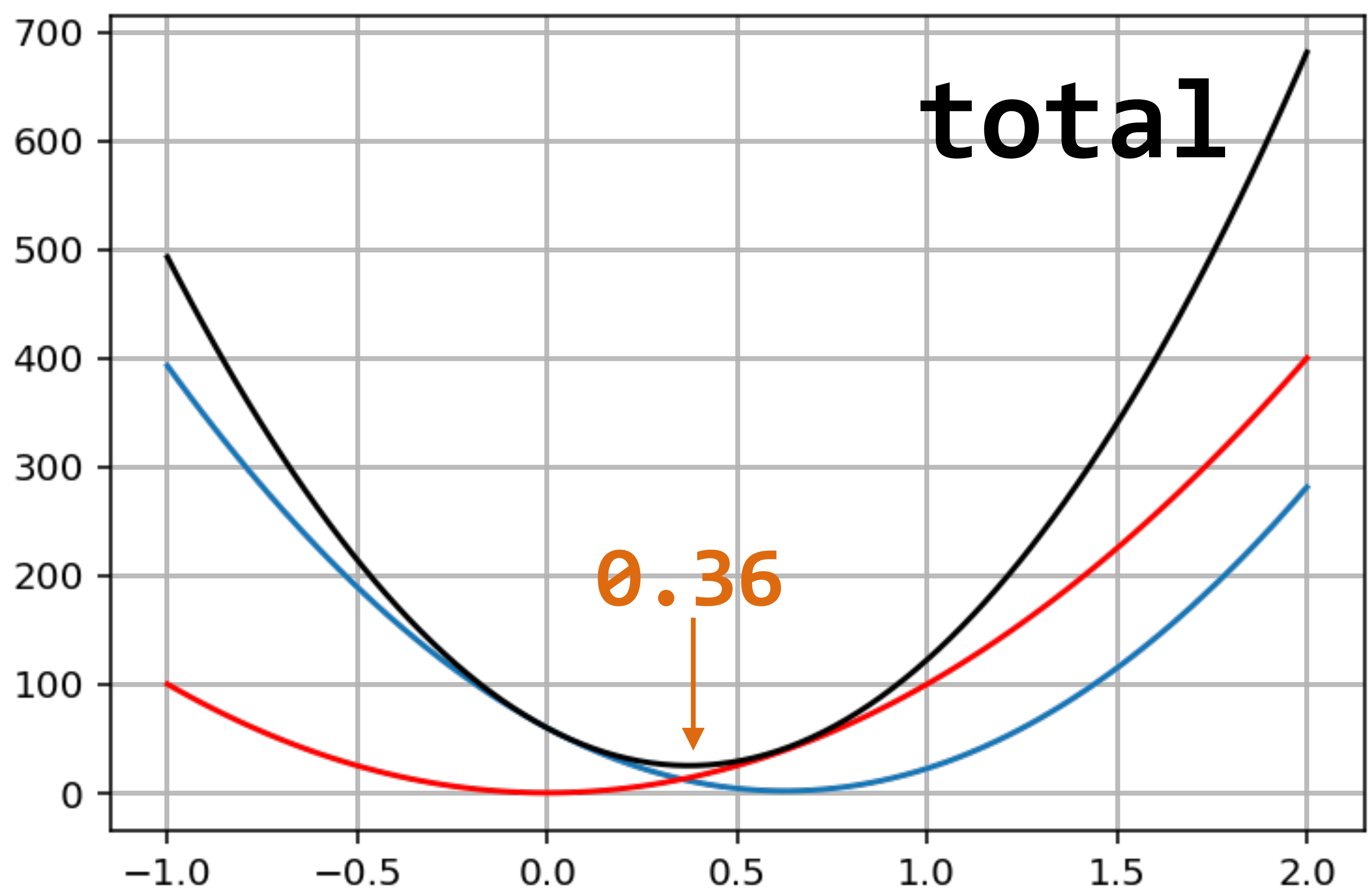

beta

COVARIANCE

* A measure of the “joint variability” of two variables

COVARIANCE

\mbox{cov}(\vec{x},\vec{y}) = \frac{1}{n}\sum_{i=1}^n(x_i-\bar{x})(y_i-\bar{y})

\mbox{cov}(X,Y) = E[(X-E[X])(Y-E[Y])]

\mbox{cov}(X,X) = E[(X-E[X])(X-E[X])] = E[(X-E[X])^2] = \mbox{var}(X)

$$\mbox{cov}(\vec{x},\vec{y}) = \frac{1}{n}\sum_{i=1}^n(x_i-\bar{x})(y_i-\bar{y})$$

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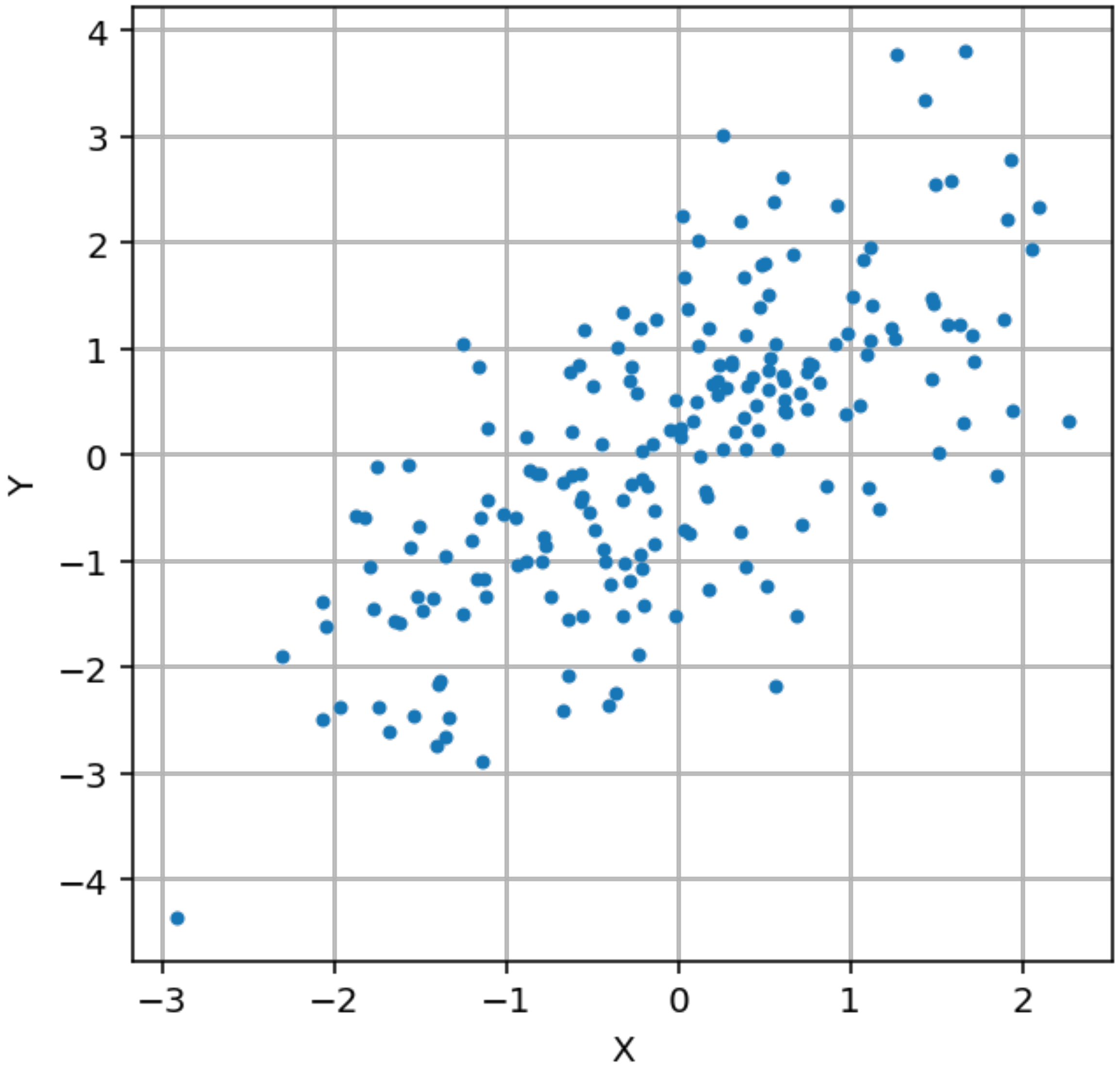
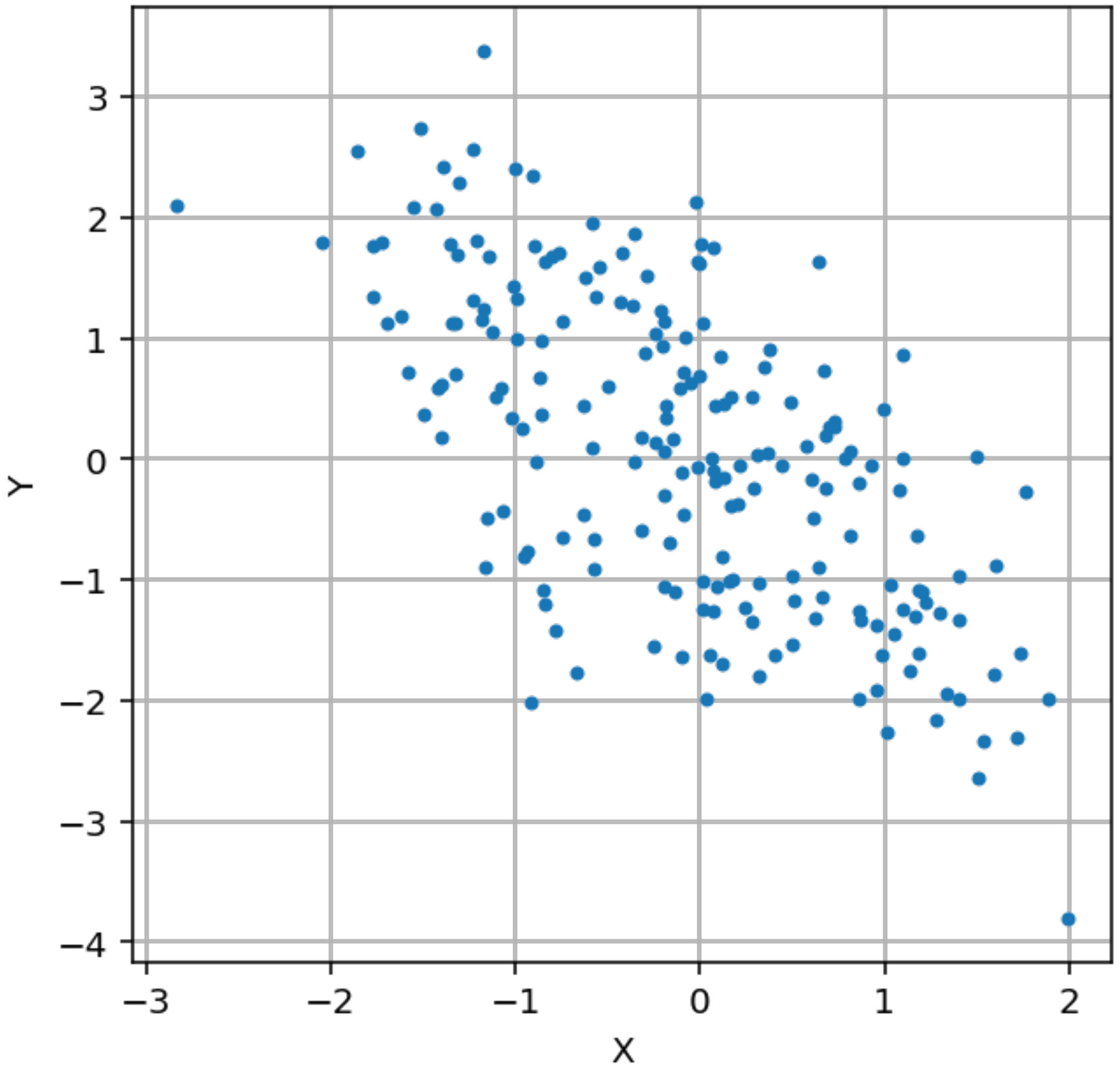
COVARIANCE



cov(x,y) > 0?

cov(x,y) < 0?

COVARIANCE

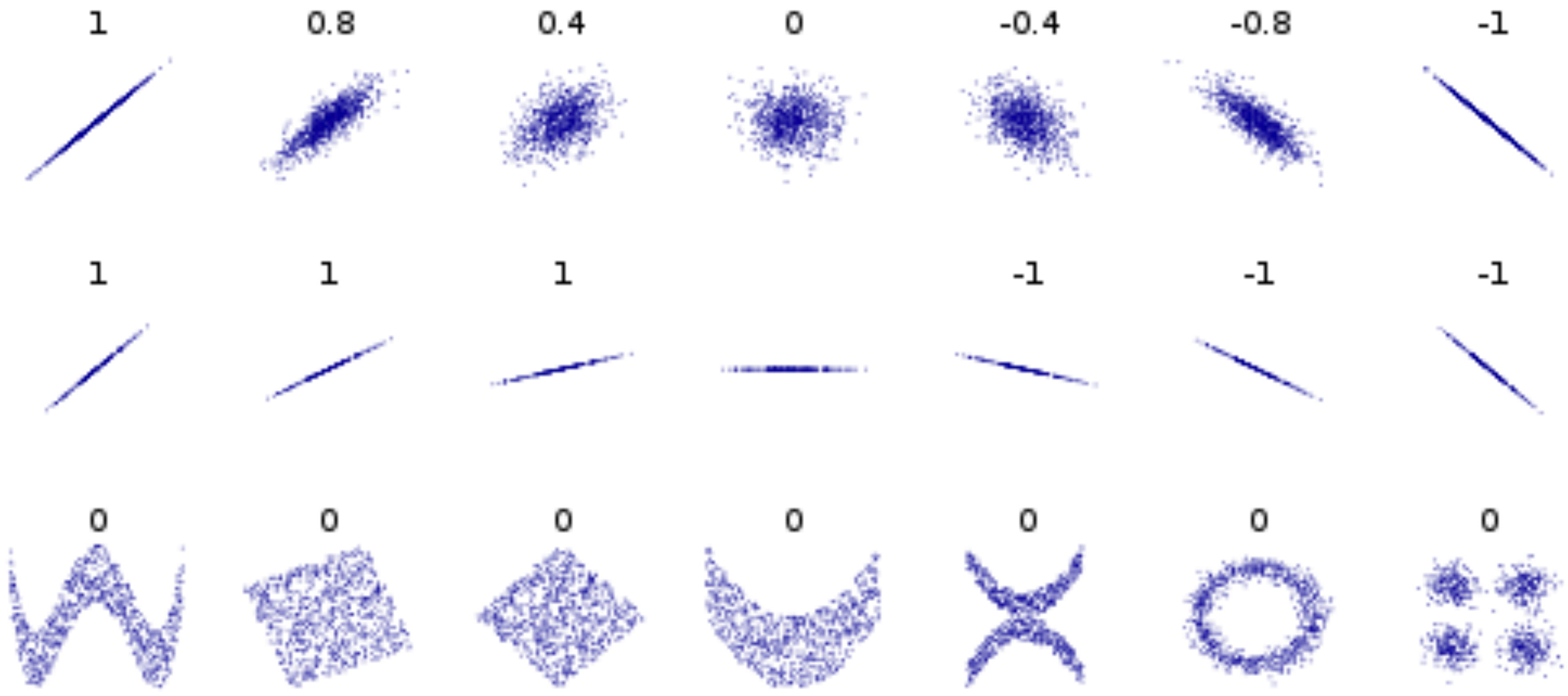


`cov(x,y) > 0?`

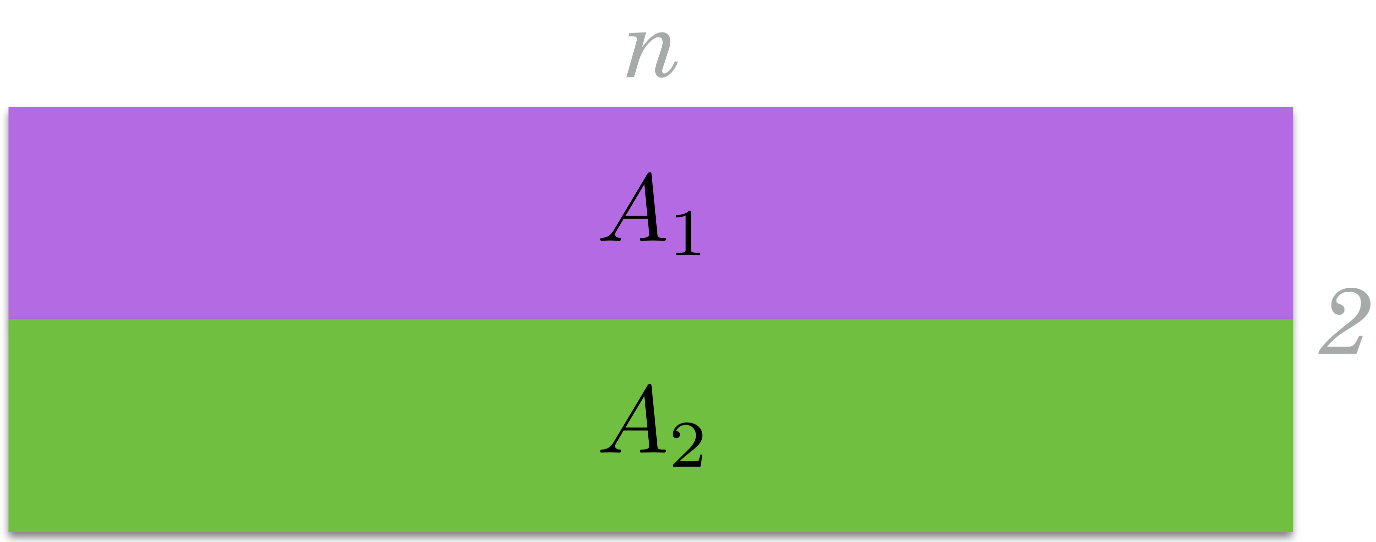
`cov(x,y) < 0?`

COVARIANCE

(Well, correlation…)



COVARIANCE MATRIX

$A =$ 

$$\text{cov}(A) = \begin{bmatrix} \text{var}(A_1) & \text{cov}(A_1, A_2) \\ \text{cov}(A_1, A_2) & \text{var}(A_2) \end{bmatrix}$$

(assuming A is mean 0)

$$\text{cov}(A) = \left(\frac{1}{n}\right) A A^T$$

\mbox{cov}(A) = \begin{bmatrix}
\mbox{var}(A_1) & \mbox{cov}
(A_1,A_2) \\ \mbox{cov}(A_1,A_2
\mbox{var}(A_2) \end{bmatrix}

\mbox{cov}(A) = \left(\frac{1}{n}\r
A A^T

TIKHONOV REGRESSION

\hat\beta = \underset{\beta}{\mbox{argmin}} \left[||Y-X\beta||_2^2 + \lambda ||\beta||_2^2 \right]

\hat\beta = \underset{\beta}

$$Y = X\beta + \epsilon$$

* RIDGE REGRESSION

$$\hat{\beta} = \underset{\beta}{\text{argmin}} \left[||Y - X\beta||_2^2 + \lambda ||\beta||_2^2 \right]$$

ERROR or LOSS PENALTY

* TIKHONOV REGRESSION

$$\hat{\beta} = \underset{\beta}{\text{argmin}} \left[||Y - X\beta||_2^2 + \lambda ||C\beta||_2^2 \right]$$

PENALTY MATRIX

TIKHONOV REGRESSION

* RIDGE REGRESSION is a special case of TIKHONOV REGRESSION

* TIKHONOV REGRESSION puts a **ZERO-MEAN MULTIVARIATE NORMAL PRIOR** on the weights

* in RIDGE REGRESSION the covariance matrix of the prior has a constant diagonal

    * i.e. the prior is a **SPHERE**

* in TIKHONOV REGRESSION the covariance matrix can be <u>***ANYTHING***</u>

TIKHONOV REGRESSION

* the multivariate normal prior given by **TIKHONOV REGRESSION**

$$\beta \sim N(0, \sigma^2 (C^T C)^{-1})$$

\beta \sim N(0, \sigma^2 \Lambda^{-1}), \Lambda = C^T C

TIKHONOV REGRESSION

```
\begin{eqnarray*}
A &=& XC^{-1}\\
\hat\beta_A &=& \un
{\mbox{argmax}} \lef
+ \lambda ||\beta||_2
```

* any **TIKHONOV** problem can be converted into a **RIDGE** problem

$$A = XC^{-1}$$ ← **1. CHANGE OF BASIS**

$$\hat{\beta}_A = \underset{\beta}{\text{argmin}} \left[||Y - A\beta||_2^2 + \lambda ||\beta||_2^2 \right]$$

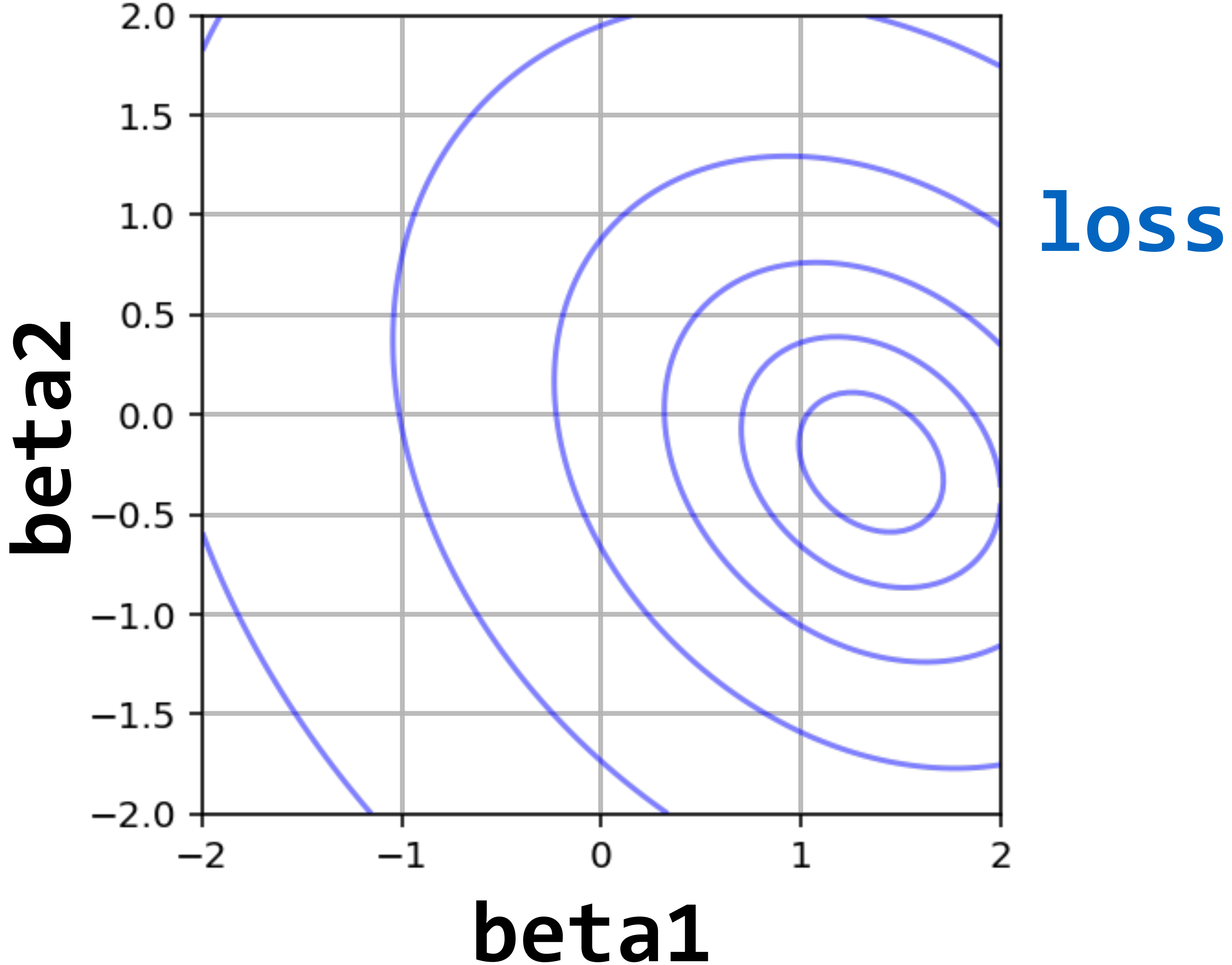
↑ **2. RIDGE REGRESSION**

$$\hat{\beta} = C^{-1}\hat{\beta}_A$$ ← **3. CHANGE BASIS AGAIN**

Rank-Deficient and Discrete Ill-Posed Problem: Numerical Aspects of Linear Inversion (1998; Per Christian Hansen)

EXAMPLE

$$y_t = x_{1,t}\beta_1 + x_{2,t}\beta_2$$



EXAMPLE

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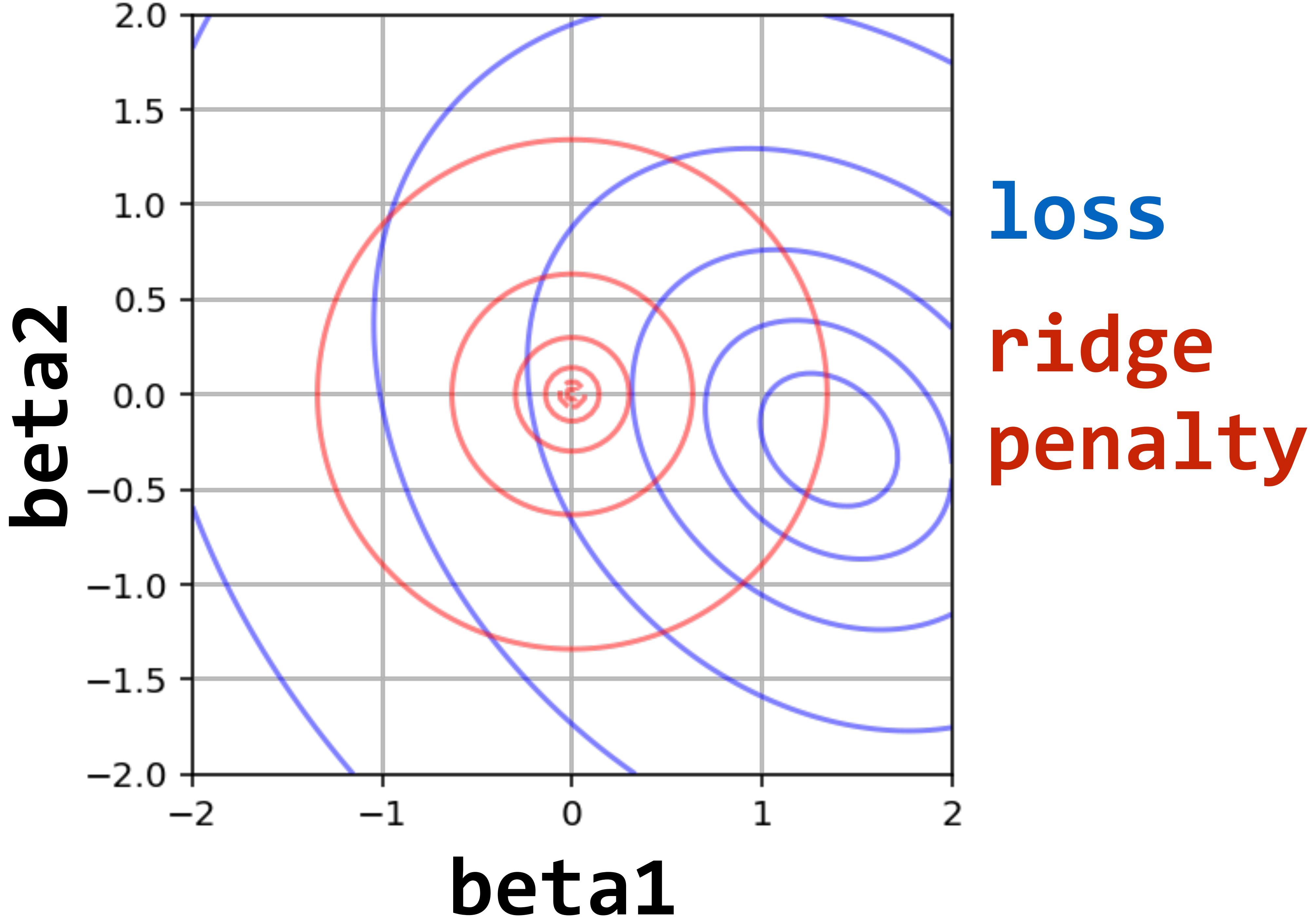

EXAMPLE

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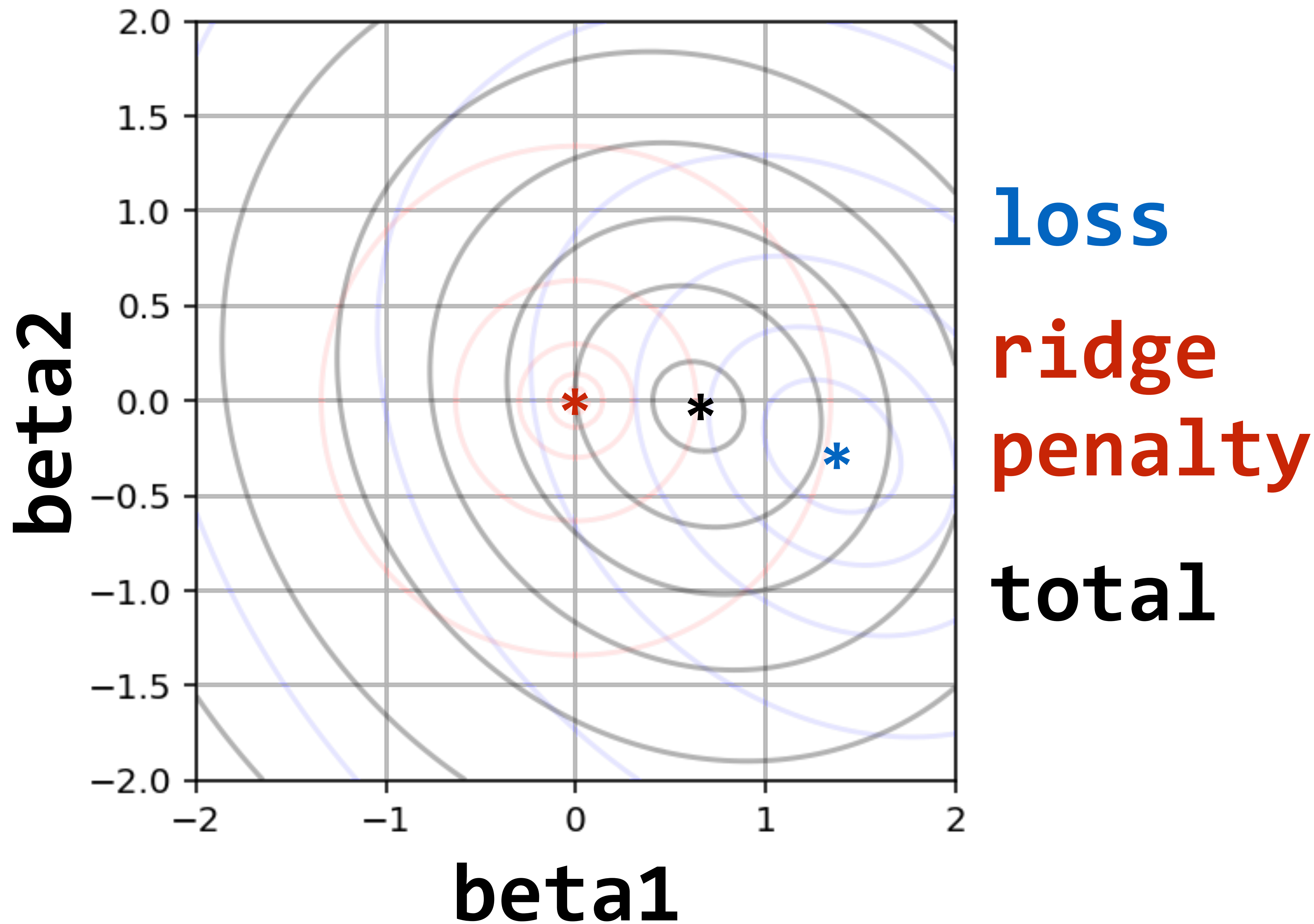
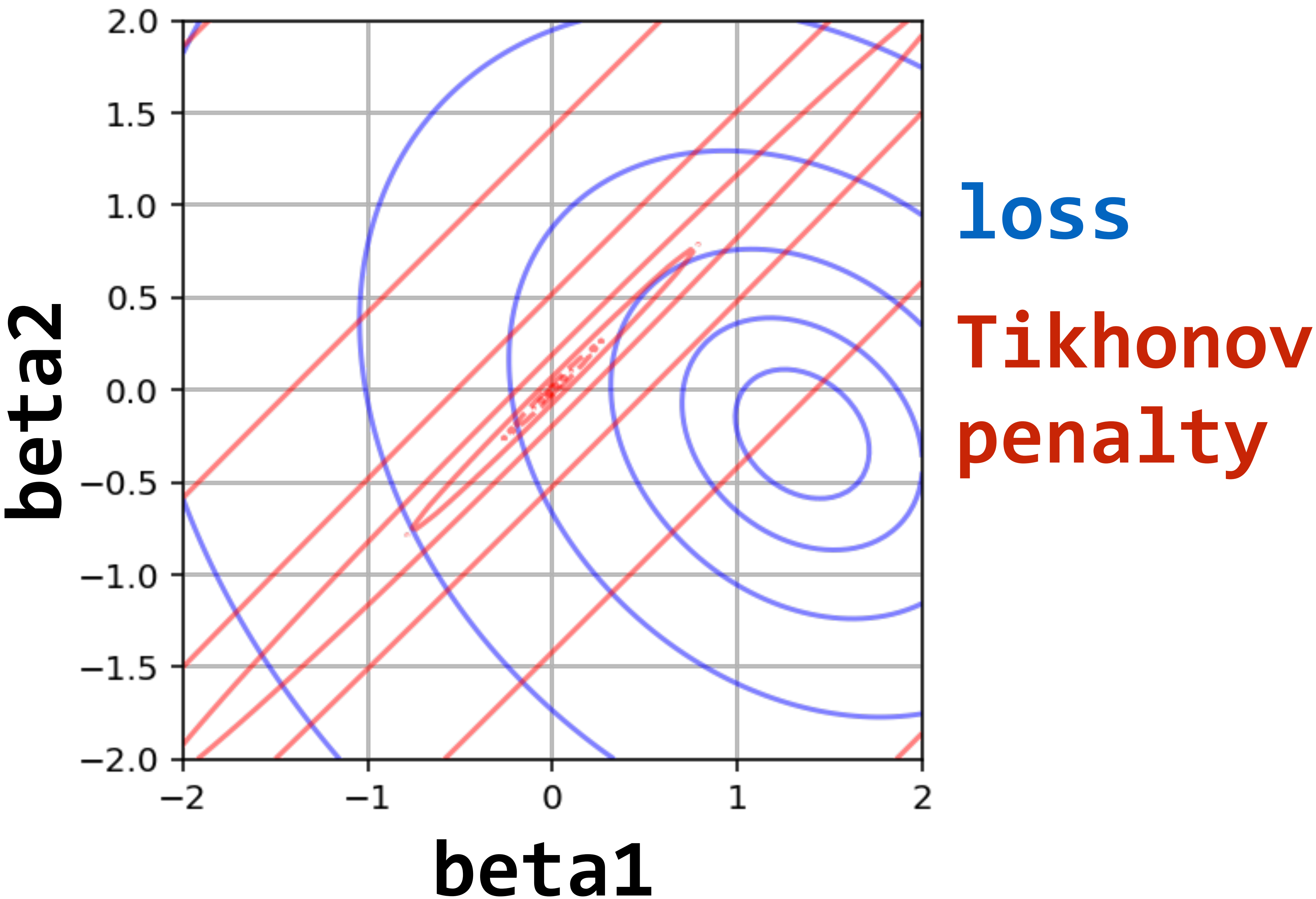


EXAMPLE

* Suppose we strongly suspect that **beta1** and **beta2** should be similar

EXAMPLE

$$y_t = x_{1,t}\beta_1 + x_{2,t}\beta_2$$



EXAMPLE

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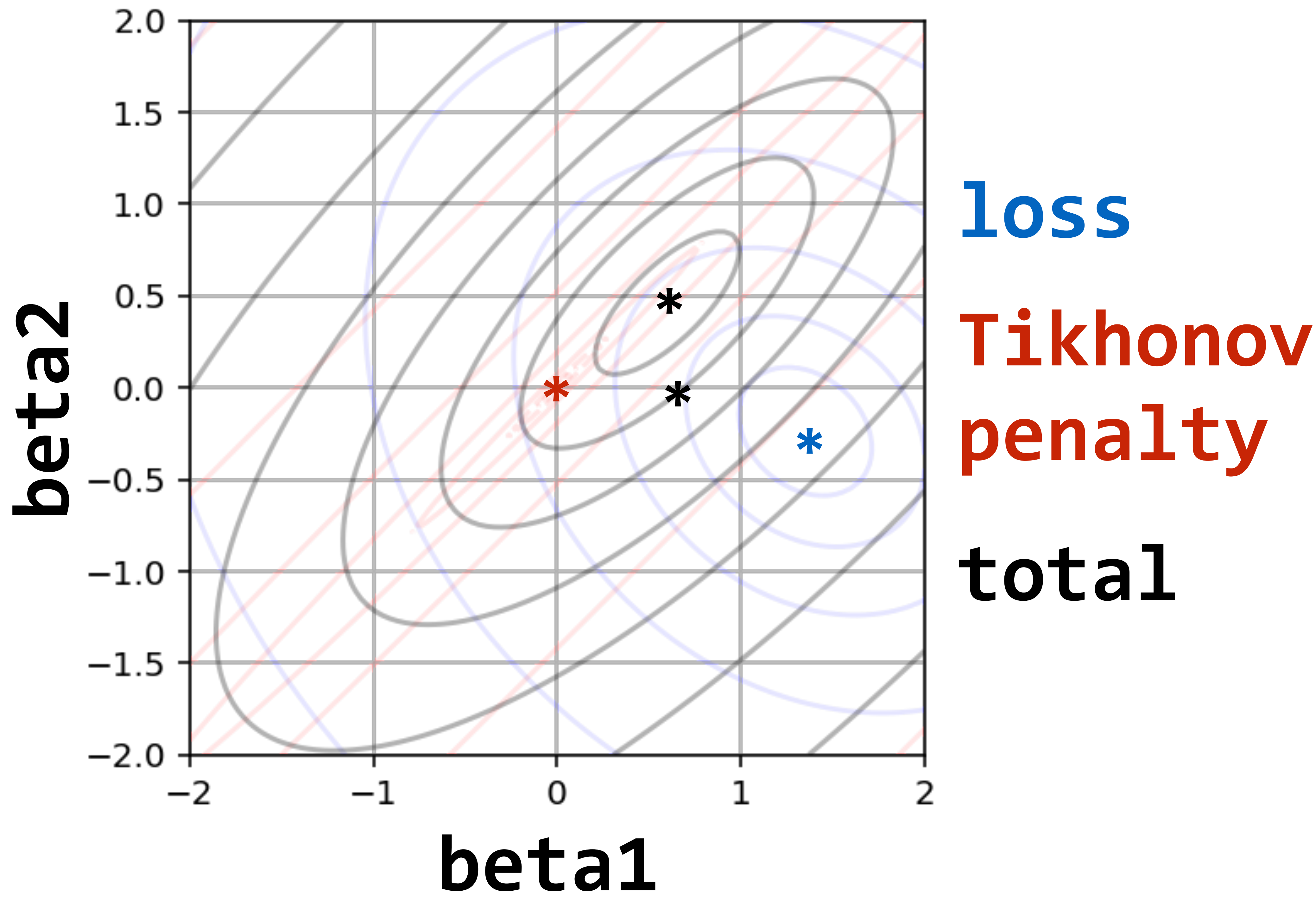


TIKHONOV REGRESSION

* any **TIKHONOV** problem can be converted into a **RIDGE** problem by a **LINEAR TRANSFORMATION**

* conversely, **ANY LINEAR TRANSFORMATION** of X followed by **RIDGE REGRESSION** is equivalent to some **TIKHONOV REGRESSION** problem

TIKHONOV REGRESSION

* WORD EMBEDDING MODELS

* think of stimulus matrix as **WORDS** over time projected onto WORD EMBEDDING

WORDS EMBEDDING

$$\underset{t\times n}{X} = \underset{t\times w}{W}\underset{w\times n}{E}$$

TIME WORDS EMBEDDING DIMENSIONS

\underset{t\times n}{X} = \underset{t\times w}{W} \underset{w\times n}{E}

TIKHONOV REGRESSION

* this is equivalent to **TIKHONOV REGRESSION** on the **WORDS** with a prior determined by the **WORD EMBEDDING**

$$\underbrace{\frac{1}{\sigma^2}\Sigma_\beta}_{\text{PRIOR COVARIANCE}} = \underbrace{(C^T C)^{-1}}_{\text{INVERSE OF PENALTY INNER PRODUCT}} = \underbrace{E^T E}_{\text{EMBEDDING INNER PRODUCT}}$$

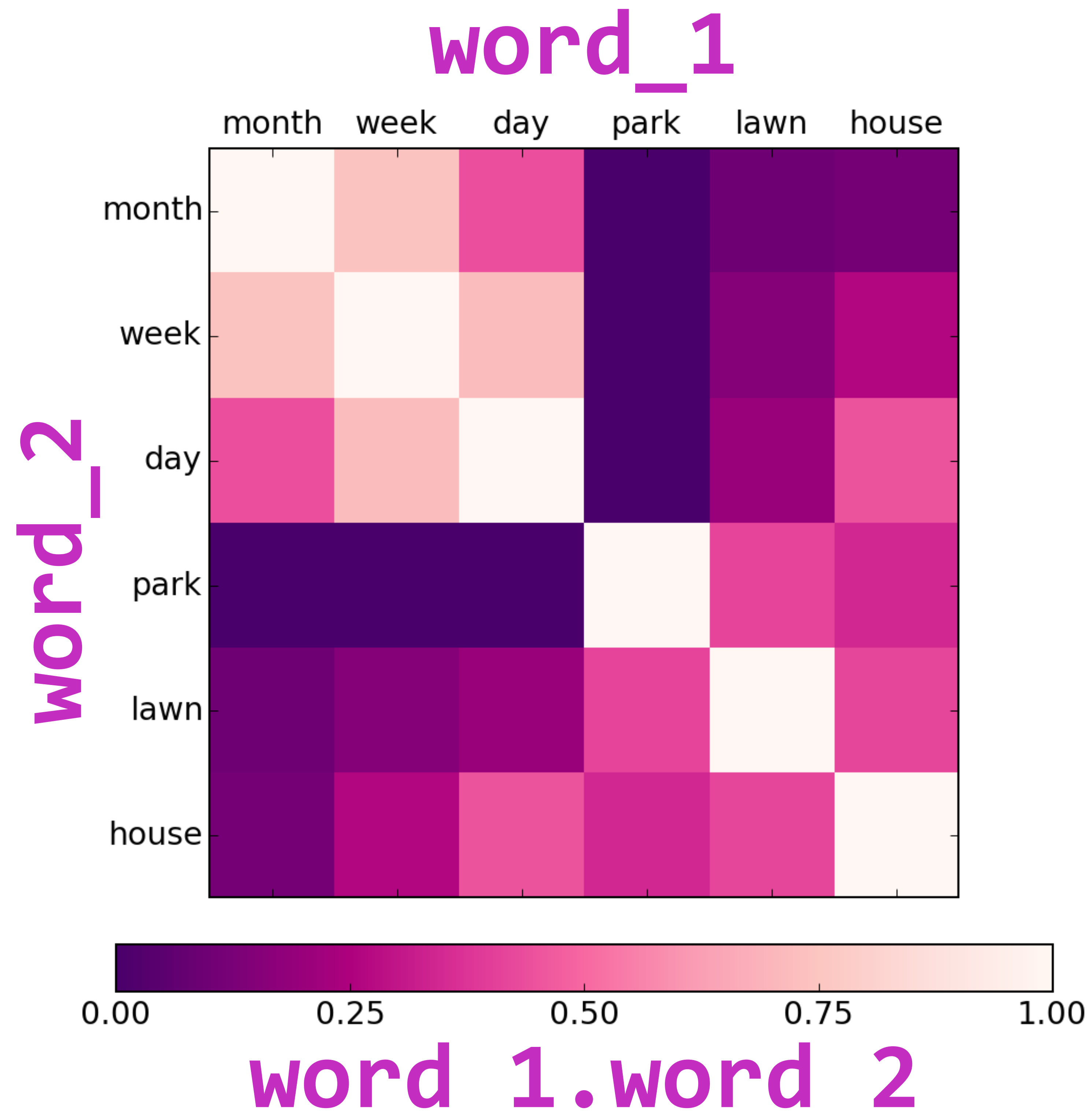
* **i.e. the prior covariance between two words' weights is equal to the dot product of their embedding vectors**

\frac{1}{ \sigma^2
\Lambda^{-1} = E

TIKHONOV REGRESSION

$$E^T E =$$

EMBEDDING INNER PRODUCT, ***english1000***



TIKHONOV REGRESSION

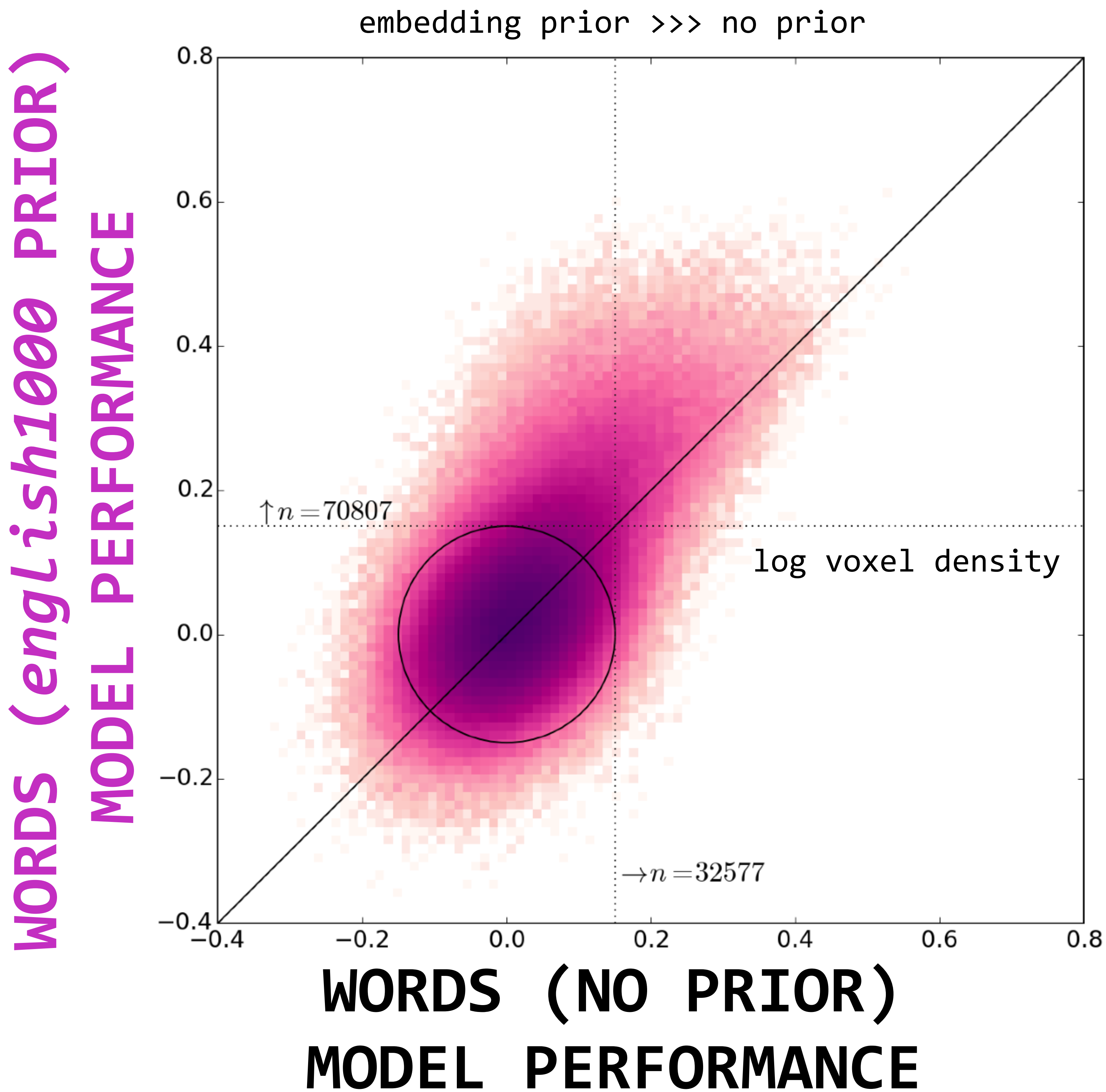
\underset{w \times v}
\underset{w \times n}
\underset{n \times v}{

* to get **WEIGHTS ON WORDS** we just project onto the **EMBEDDING**

$$\underset{w \times v}{\overset{\text{WEIGHTS IN WORD SPACE}}{\hat{\beta}_W}} = \underset{w \times n}{\overset{\text{EMBEDDING}}{E}} \; \underset{n \times v}{\overset{\text{WEIGHTS IN EMBEDDING SPACE}}{\hat{\beta}_X}}$$

* (this is equivalent to simulating responses to single words)

TIKHONOV REGRESSION



NEXT TIME

* Data quality!